



# Gasoline Combustion Fundamentals

Isaac Ekoto  
Sandia National Laboratories

2017 DOE Vehicle Technologies Office Annual Merit Review  
Washington, DC  
June 6, 2017 – 1:45 p.m.

Program Manager: Leo Breton & Gurpreet Singh  
U.S. DOE Vehicle Technologies Office

Project ID: ACS006

This presentation does not contain any proprietary, confidential, or otherwise restricted information

# Overview

## Timeline

- Project provides fundamental research supporting DOE/industry advanced engine development projects.
- Project directions and continuation are evaluated annually.

## Budget

- Project funded by DOE/VTO
- FY17 funding: \$700K

## Barriers identified in VTO Multi-Year Program Plan

- Insufficient knowledge base for advanced LTC or mixed-mode combustion systems over the full load range
- Models are needed for fundamental engine combustion and in-cylinder emissions formation processes
- Lack of effective engine control for advanced lean-burn direct injection gasoline engine technology

## Partners

- Project lead: Isaac Ekoto, Sandia National Laboratories
- Industry/Small Business Partners:
  - GM, Ford, & FCA: technical guidance
  - 15 Industry partners in DOE Working Group
  - Mahle GmbH
  - Transient Plasma Systems Inc.
- University/National Lab Collaborators:
  - Argonne National Lab: Low-temperature plasma modeling
  - U. Minnesota: Engine sample speciation
  - U. Orléans (France): In-cylinder ozone generation
  - Michigan State University: Turbulent jet ignition



# Relevance & Objectives

## Project Objective:

- Expand the fundamental understanding of fluid-flow, thermodynamics, and combustion processes needed to achieve clean and efficient gasoline engines

## FY17 Objectives:



- Explore how low-temperature plasma (LTP) igniters can facilitate efficient, mixed-mode combustion across the load/speed map:
  - Low load/speed: In-cylinder ozone generation for controllable **LTGC**
  - Moderate load/speed: Extended dilution tolerances for **lean-burn SI**
  - High load: Improved knock resistance for **boosted SI**
- Improve foundational knowledge base of LTP ignition mechanisms through well-controlled experiments and modeling
- Benchmark LTP igniter performance in an optically accessible DISI engine
- Create hardware needed to evaluate pre-chamber igniter physics and in-cylinder performance metrics

## Impact

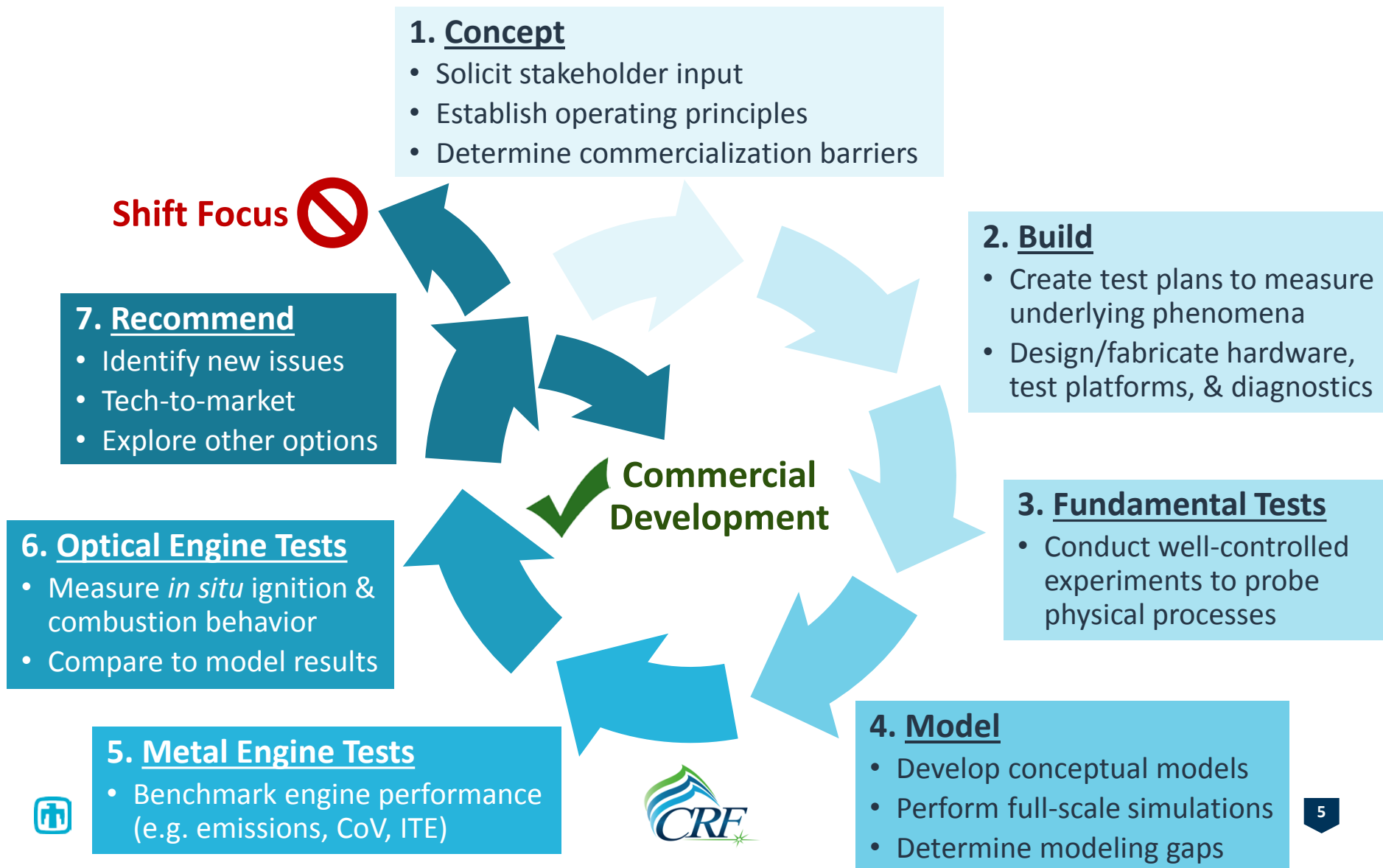
- Better understanding of igniter physics enables predictive simulation ignition model development and provides insight on hardware/operating strategy optimization for mixed-mode combustion



# FY17 Milestones

<u>Quarter</u>	<u>Milestone</u>	<u>Status</u>
Q1	Measure low-temperature plasma generated radicals in the optical calorimeter with representative fuel and EGR compositions.	
Q2	Benchmark DISI emissions and combustion performance metrics for different low-temperature plasma igniter configurations.	
Q3	Perform high-speed and spectroscopic imaging of low-temperature plasma igniters in the optically-accessible engine during ignition.	<b>In Progress</b>
Q4	Develop a suitable research engine head for turbulent jet ignition experiments.	<b>In Progress</b>

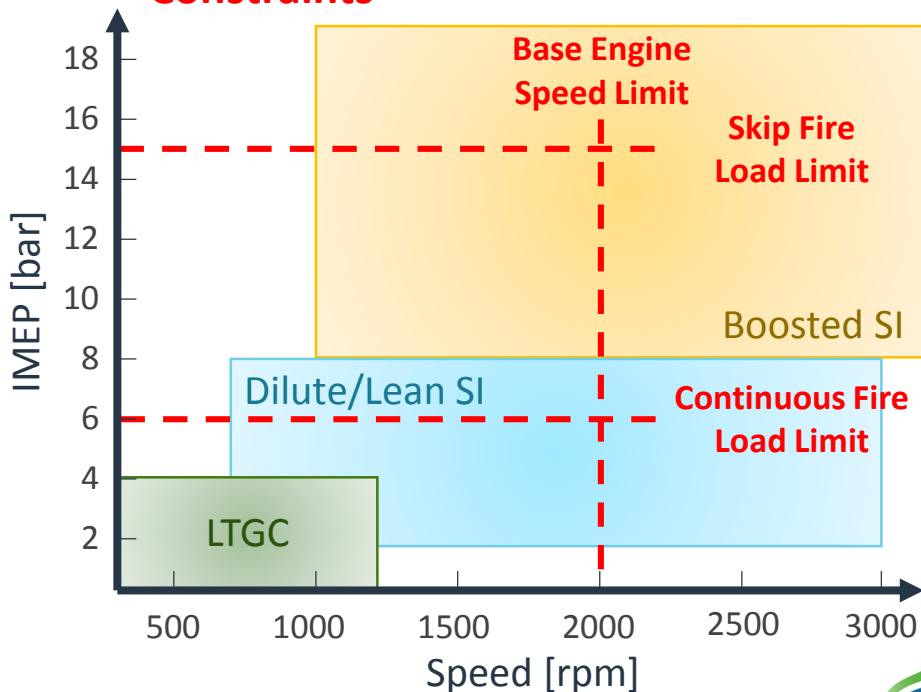
# Approach: Remove new igniter commercialization barriers



# Approach: Operating regime and test equipment

	Low-Temperature Gasoline Combustion	Un-throttled SI (lean or dilute)	Stoichiometric Boosted SI
Benefits	$\uparrow \eta_{TE}$ , $\uparrow \eta_{vol}$ , $\downarrow Q_{HT}$ , $\downarrow T_{ad}$	$\uparrow \eta_{TE}$ , $\uparrow \eta_{vol}$ , $\downarrow Q_{HT}$ , $\downarrow T_{ad}$	$\uparrow \eta_{mech}$ , $\downarrow Q_{HT}$
Challenges	$\uparrow COV$ , $\uparrow HC/CO$ , $\uparrow P_{peak}$ , $\uparrow dP/dt$	$\uparrow COV$ , $\uparrow HC/CO$	$\uparrow P_{peak}$ , $\uparrow dP/dt$ , LSPI, Knock
Desired ignition characteristics	Chemically controlled auto-ignition centered near TDC	Multiple ignition sites with fast early flame propagation	Stable ignition with significant spark retard

## Constraints



Assumptions: Variable valve lift/timing, Central DI, CR > 12

	Old Engine	New Engine		
Combustion Mode	LTGC	LTGC	Dilute SI	Boosted SI
Head design	3 valve pent-roof	4-valve pent-roof		
Igniter	None	Centrally mounted LTP		
Displacement [L]	0.63	0.55		
Stroke/Bore	1.03	1.11		
CR	11.3	13		
Intake P [bar]	1	0.8 – 1.2		1 – 2
Valve Timing	150° NVO	~34° PVO		~7° PVO

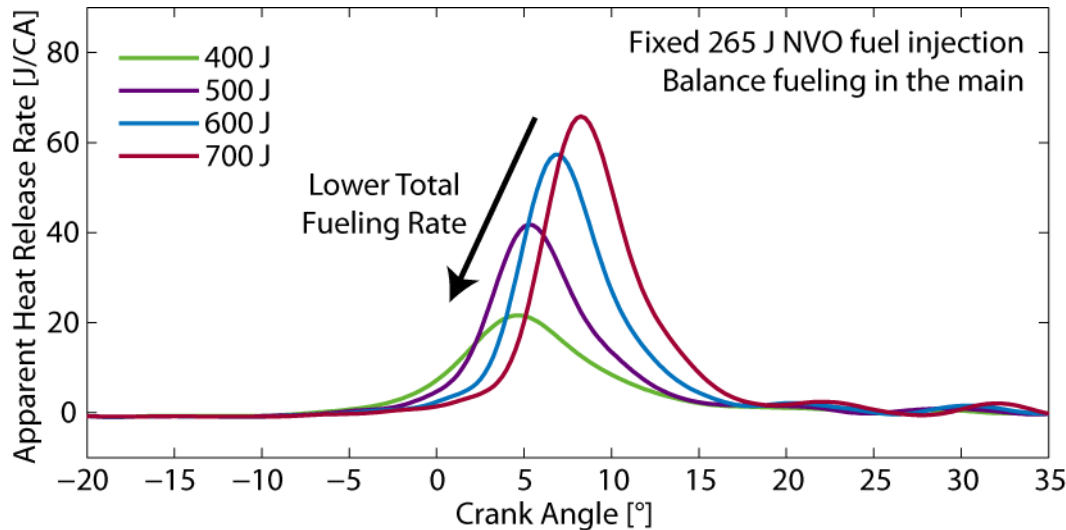
Fundamental studies: optically accessible calorimeter

- Gases: O<sub>2</sub>, N<sub>2</sub>, CO<sub>2</sub>, H<sub>2</sub>O (could add NO, gaseous HC)
- Temperature: up to 70°C
- Pressure: up to 9 bar (abs.) in current config.
- Measurable ΔP: single-digit Pascals (29 cc chamber)
- Other diagnostics: imaging, schlieren, absorption, LIF



# Previous: Impact of NVO reformat on LTGC auto-ignition

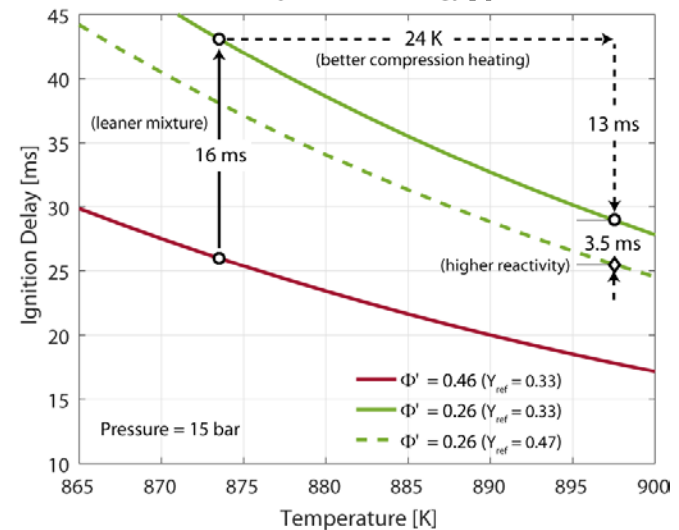
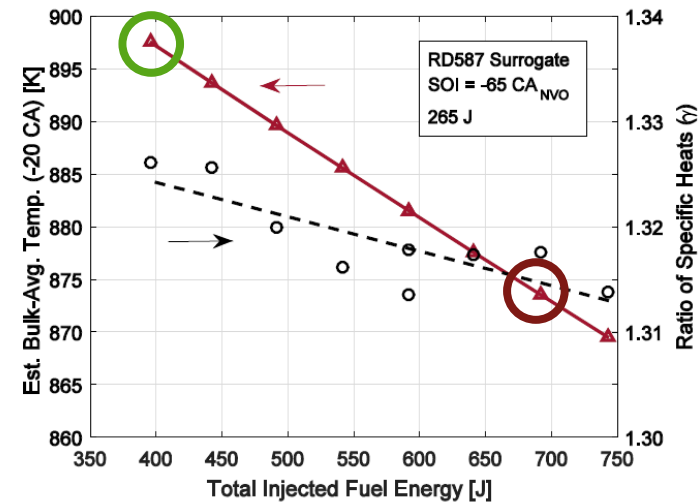
Ekoto et al, ASME ICEF 2016-9458



Competing effects examined via chemical modeling:

- auto-ignition retards for leaner  $\phi$
- **higher bulk temp.** from  $\downarrow$  charge cooling &  $\uparrow \gamma$
- **increased reactivity** w/  $\uparrow$  reformat fraction
- species responsible for reactivity enhancement: acetylene, allene, acetaldehyde, & propene

**Impact: Reformate addition mechanisms that accelerate auto-ignition identified**

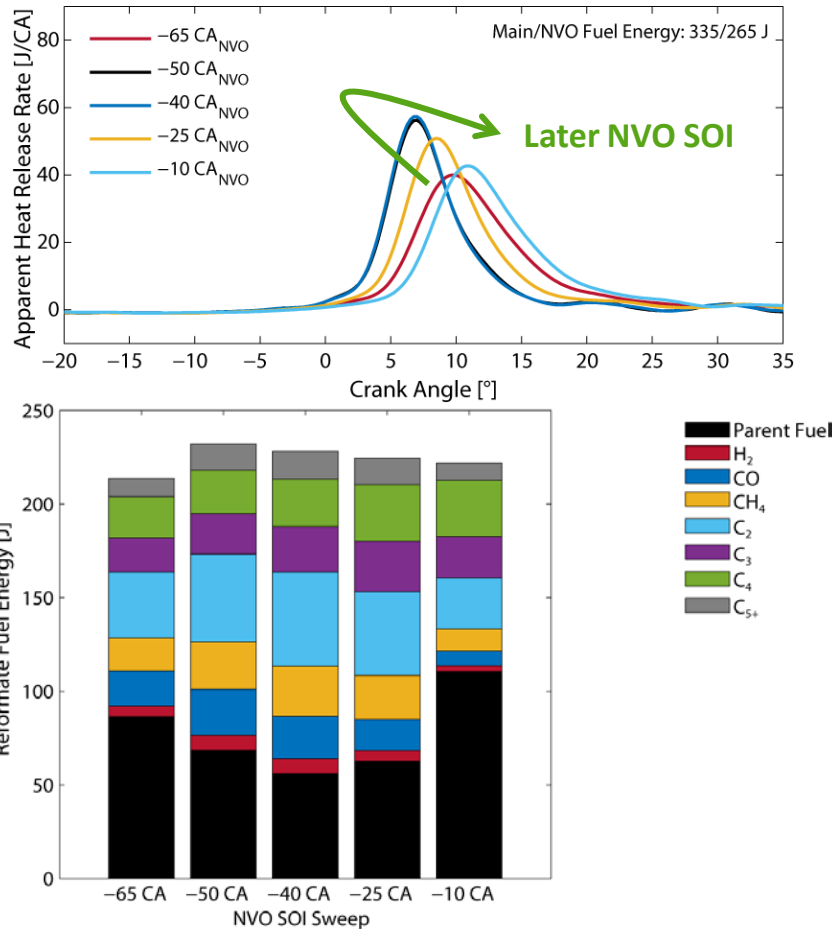


USCAR 2016 Highlight



Model

# Accomplishment: Impact of NVO reformat on LTGC



Engine Tests



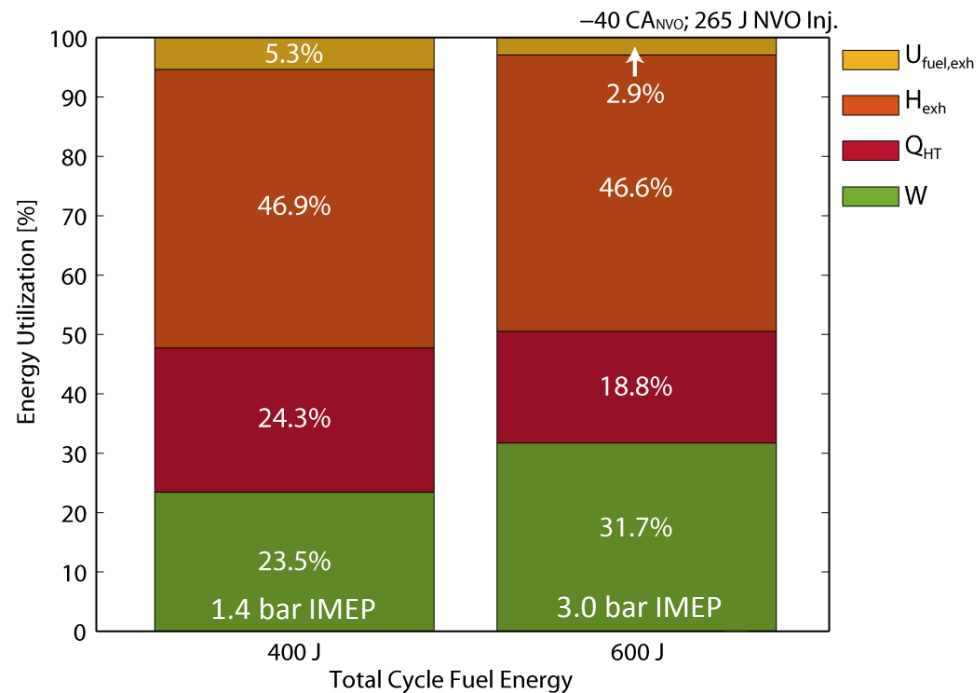
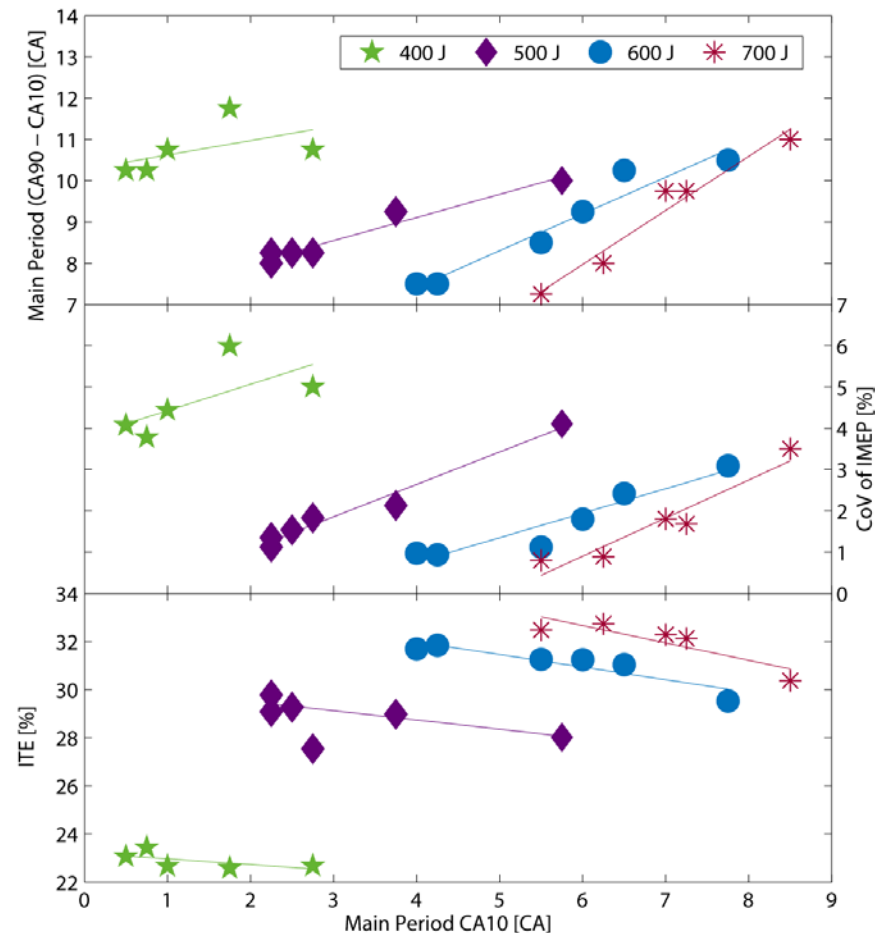
# Accomplishment: Impact of NVO reformat on LTGC

For a fixed fueling rate, as CA10 retards:

- ↓ ITE
- ↑ CoV of IMEP
- ↑ Combustion Duration



Main combustion depends on ignition delays & fueling rates (i.e. not reformat composition)



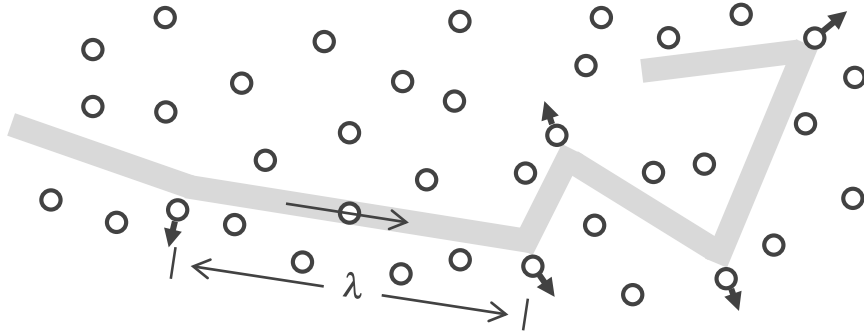
Excessive NVO-period heat loss (4-6%)

**Impact: Combustion optimally phased by altered reactivity, but heat losses are prohibitive.**



Shift Focus

# Previous: LTP igniter selection



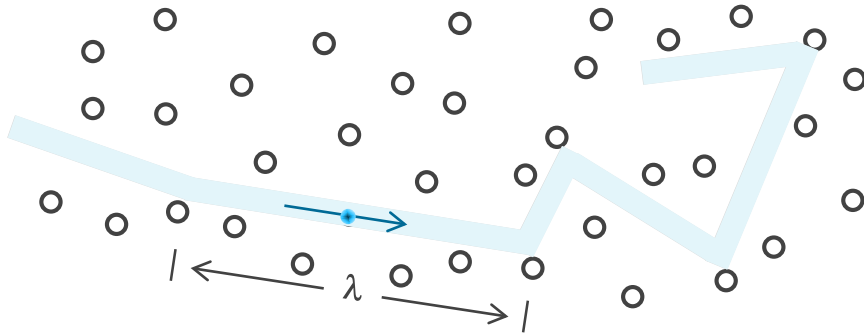
## Parameters

Mean free path:  $\lambda \propto 1/N \propto T/P$



Concept

# Previous: LTP igniter selection



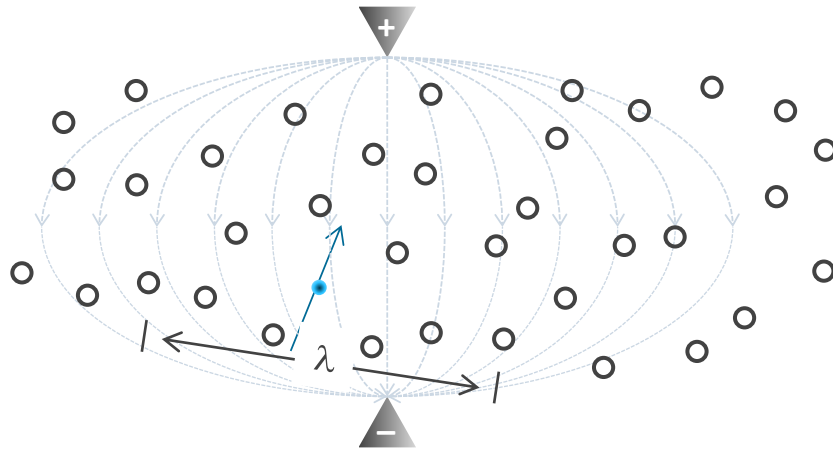
## Parameters

Mean free path:  $\lambda \propto 1/N \propto T/P$



Concept

# Previous: LTP igniter selection



## Parameters

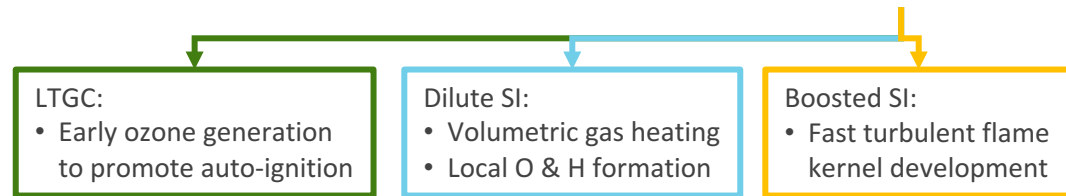
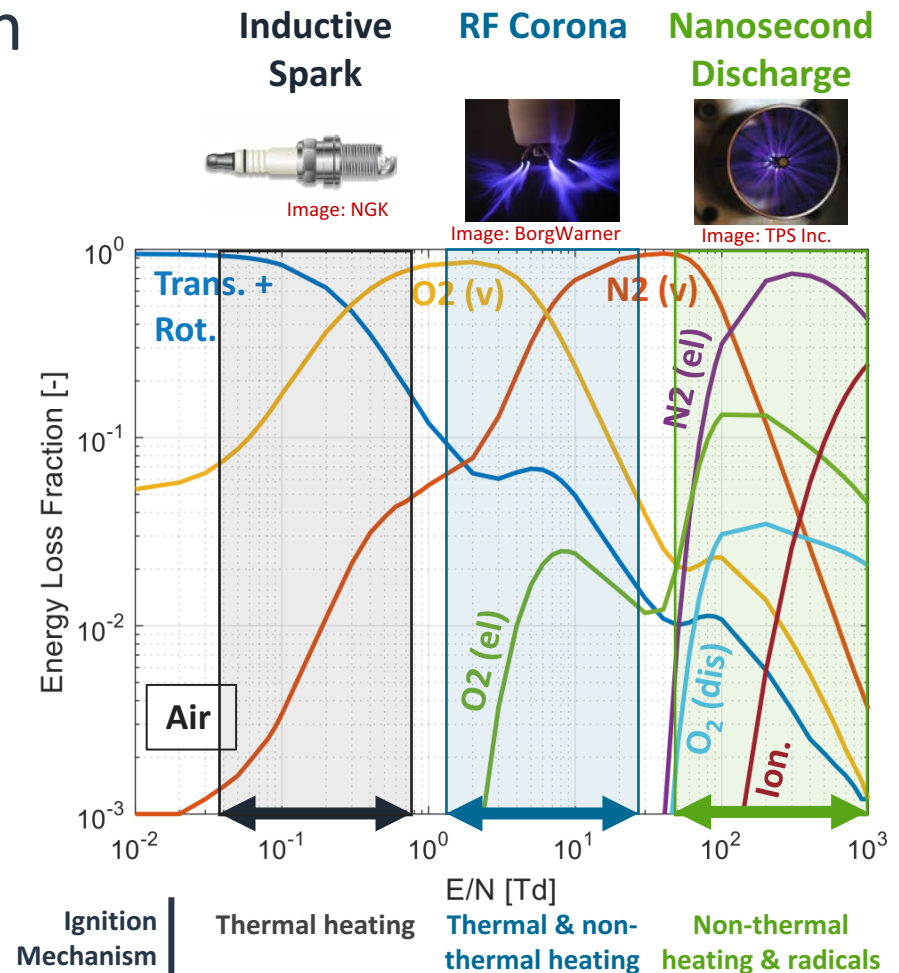
Mean free path:  $\lambda \propto 1/N \propto T/P$   
 Electric field :  $|E| \propto \text{electron acceleration}$   
 Reduced electric field:  $|E|/N \propto \text{electron energy}$

## Plasma Classification

Thermal: Elastic energy transfer  $\Rightarrow T_e \approx T_{\text{gas}}$   
 Non-thermal: Electron energy transfer  $\Rightarrow T_e \gg T_{\text{gas}}$

## Electron energy transfer mechanisms

Vibrational-to-translational relaxation: **slow**  
 Electronic gas heating: **fast**  
 Chemical ionization/dissociation: **fast**

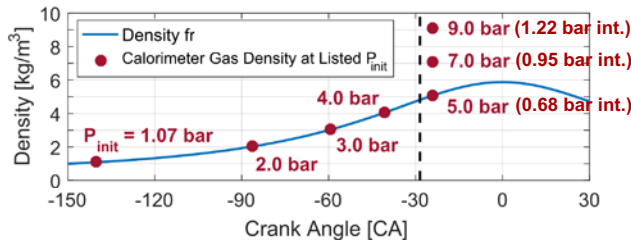


Concept

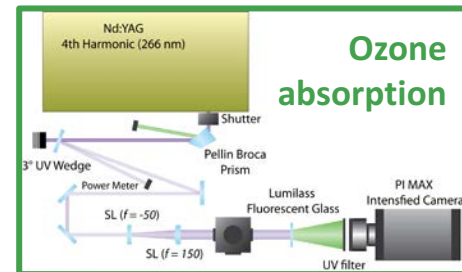
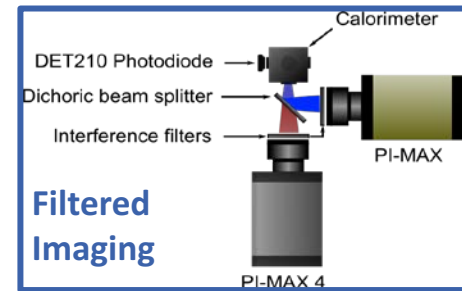
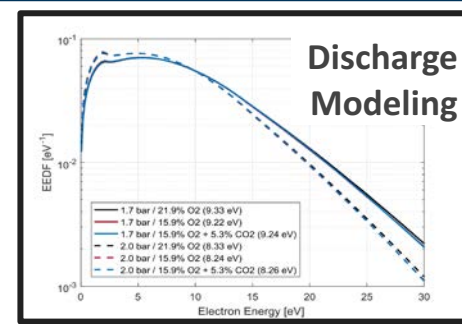
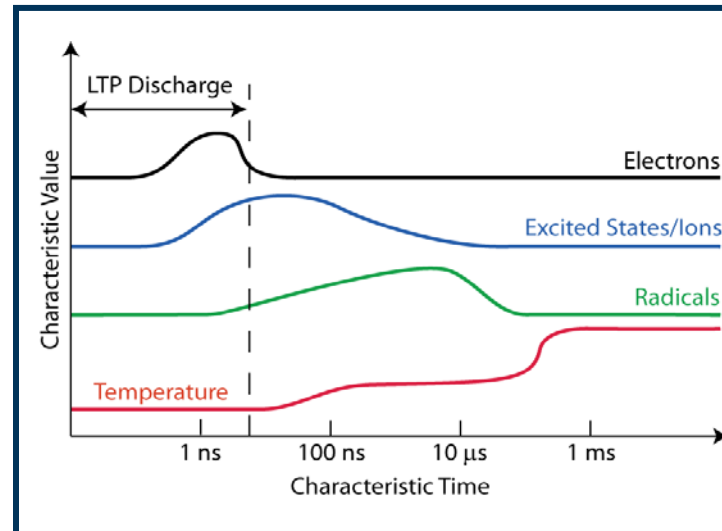
# Accomplishment: Physical LTP experiments

- High-voltage (28 kV) short duration (10 ns) pulses
- Canonical electrode geometries
  - Non-resistor spark plug
  - Ground removed & anode sharpened
  - Opposing sharpened cathode
  - Anode-only configuration also explored

Density/composition matched to Argonne single-cylinder engine tests at lean & dilution limit MBT



Sevik et al, ASME ICEF (2016)



- Pressure rise calorimetry**
- Arc Transition Probability
  - Pulse Energy
  - Electrical-to-Thermal Energy

**Impact:** Apparatus enables fundamental measurements of discharge phenomena in a well-controlled environment.

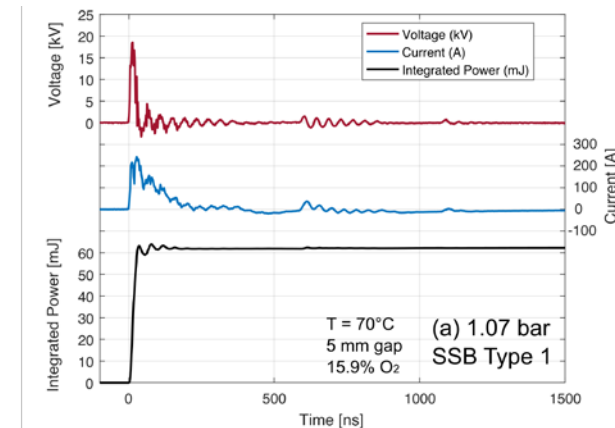
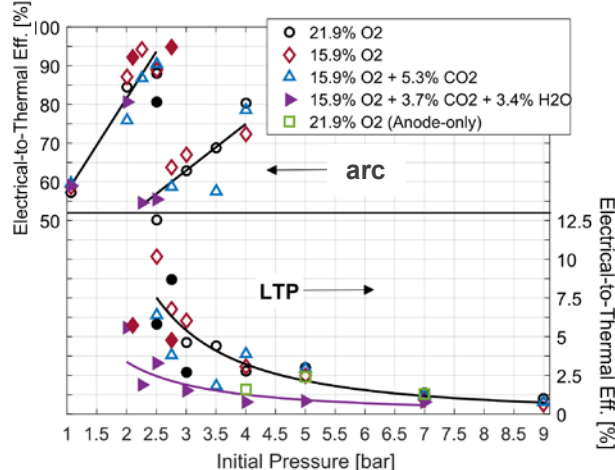
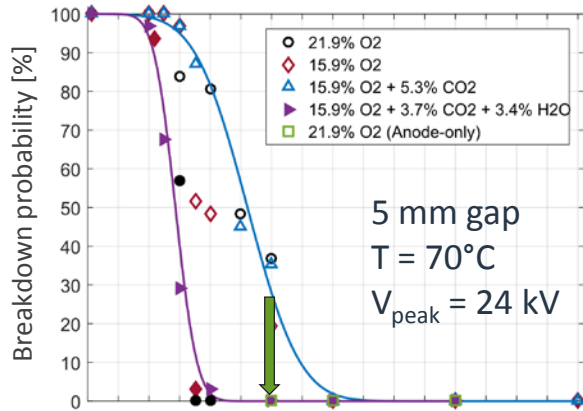


Build

# Accomplishment: Arc transition limits identified

- Minimal impact of gas composition on arc probability
- Anode-only configuration lowers the breakdown limit
  - Apparent arcs along the insulator occur at low densities
- Large reduction in breakdown transition density w/ added H<sub>2</sub>O (coincided w/ a changed in ultra-air bottle)
  - Could be lower argon content (no spec. for ultra zero air)
  - We have switched to desiccated house air
- Very efficient electric-to-thermal energy transfer during arc

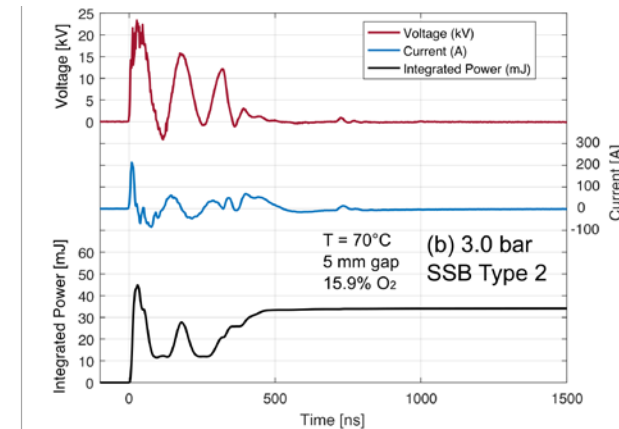
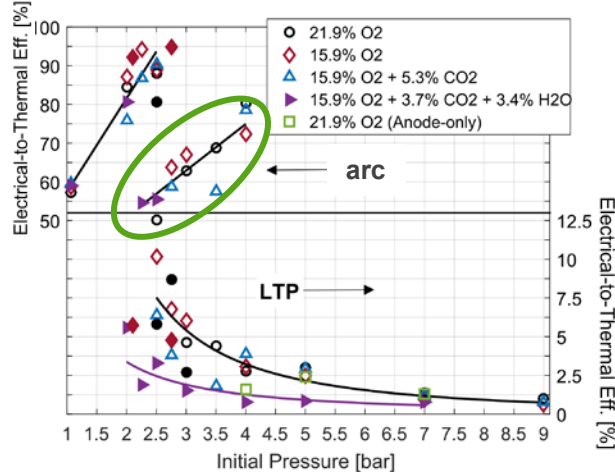
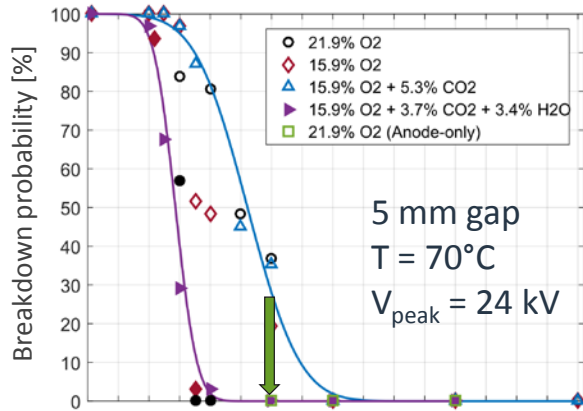
Note: solid symbols from a different ultra air bottle



# Accomplishment: Arc transition limits identified

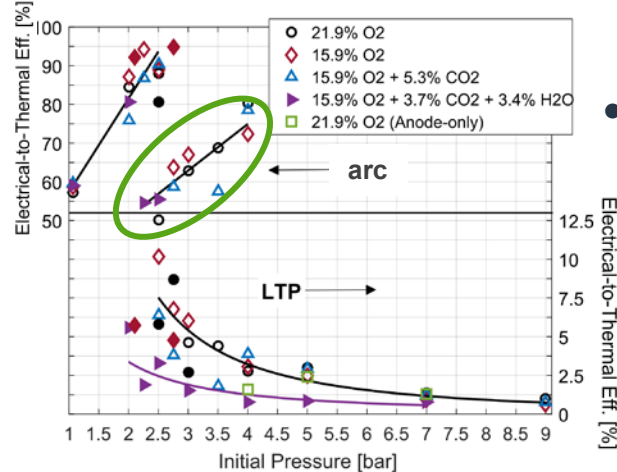
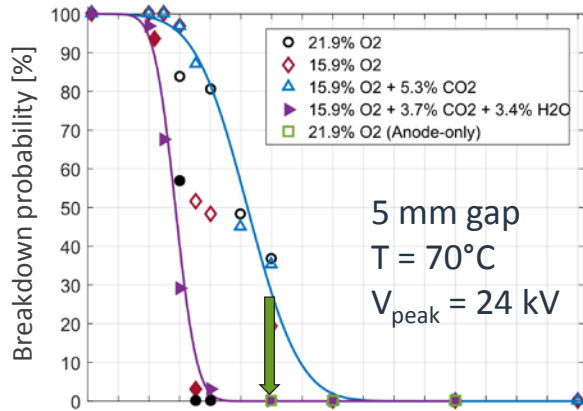
- Minimal impact of gas composition on arc probability
- Anode-only configuration lowers the breakdown limit
  - Apparent arcs along the insulator occur at low densities
- Large reduction in breakdown transition density w/ added H<sub>2</sub>O (coincided w/ a changed in ultra-air bottle)
  - Could be lower argon content (no spec. for ultra zero air)
  - We have switched to desiccated house air
- Very efficient electric-to-thermal energy transfer during arc
  - Delayed arc due to pulse voltage/current oscillations

Note: solid symbols from a different ultra air bottle

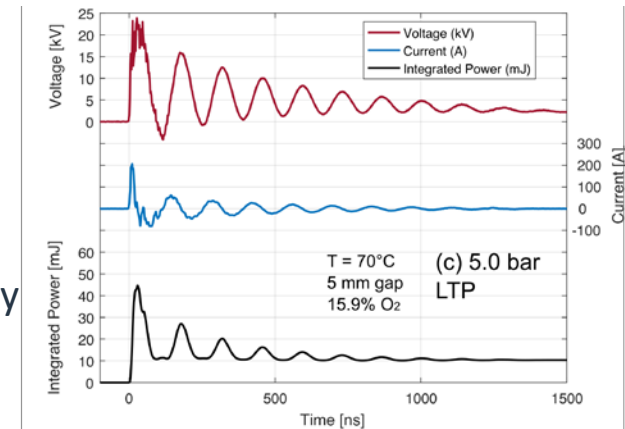


# Accomplishment: Arc transition limits identified

Note: solid symbols from a different ultra air bottle



- Minimal impact of gas composition on arc probability
- Anode-only configuration lowers the breakdown limit
  - Apparent arcs along the insulator occur at low densities
- Large reduction in breakdown transition density w/ added H<sub>2</sub>O (coincided w/ a changed in ultra-air bottle)
  - Could be lower argon content (no spec. for ultra zero air)
  - We have switched to desiccated house air
- Very efficient electric-to-thermal energy transfer during arc
  - Delayed arc due to pulse voltage/current oscillations
- Lower electric-to-thermal energy transfer for LTP
  - Exponential decay in energy transfer w/ increased density
  - Heating still comparable to inductive coil systems



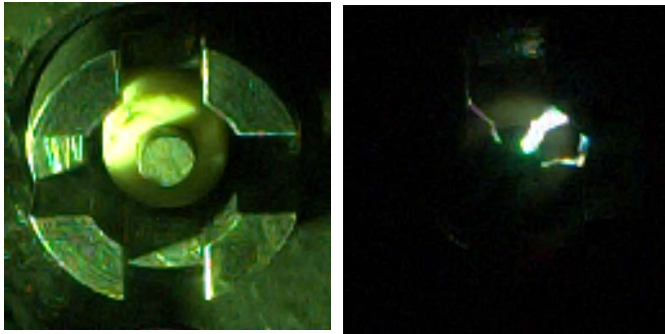
**Upshot: CO<sub>2</sub> & H<sub>2</sub>O addition to not influence occurrence of arc.**



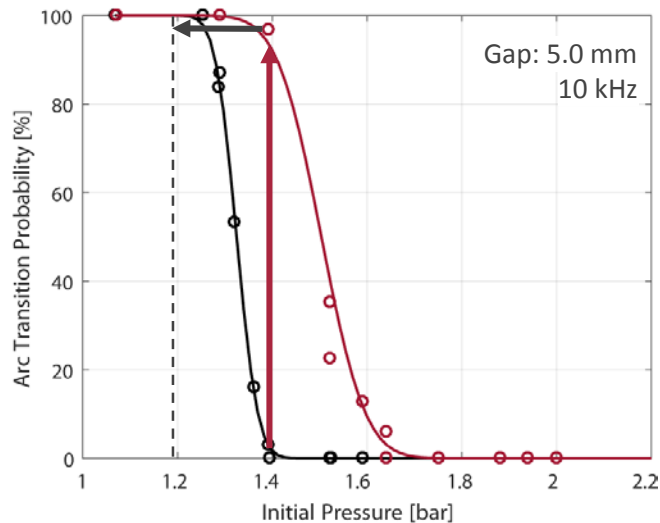


# Accomplishment: Multi-pulse arc transition explained

Sjöberg et al, SAE Int J Engines, 2014



Arcs with multi-pulse – no arc with single-pulse  
⇒ a thermal or chemical pre-conditioning mechanism



Wolk & Ekoto, IAV Conference on Ignition Systems, 2016.

Engine results confirmed by calorimetry



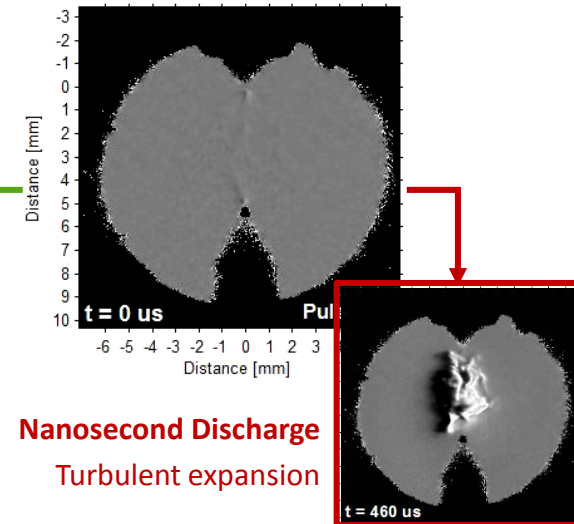
Calorimetry

$$\Delta T = \frac{E_{Thermal}}{\rho c_p V}$$

Assumed cylinder  
Thermal model  
developed

Minimal heat transfer  
between pulses

- +15% temp. @ 2<sup>nd</sup> pulse
- predicted arc probability: 100%



Inductive Spark  
Laminar expansion

Nanosecond Discharge  
Turbulent expansion

**Impact:** Extended dilution limits with nanosecond discharges attributed to arc-induced faster kernel growth rates – not LTP physics.

→ Better pulse & electrode optimization  
needed for true LTP ignition



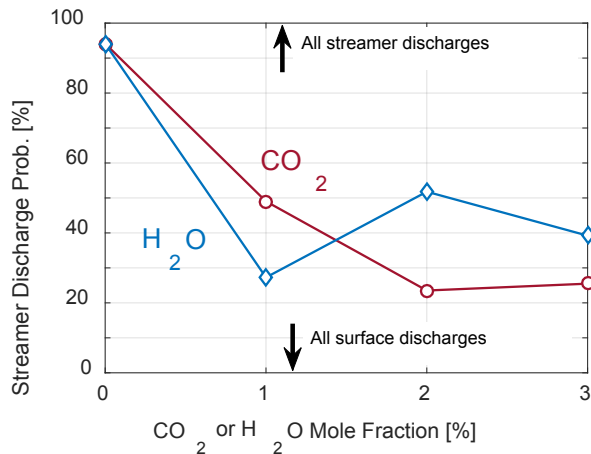
Recommend

# Accomplishment: Unique with CO<sub>2</sub>/H<sub>2</sub>O dynamics observed

- Surface discharges observed along the ceramic insulator above threshold pressure
  - Undesirable: poor heating & radical production

## CO<sub>2</sub> and H<sub>2</sub>O addition impacts discharge characteristics

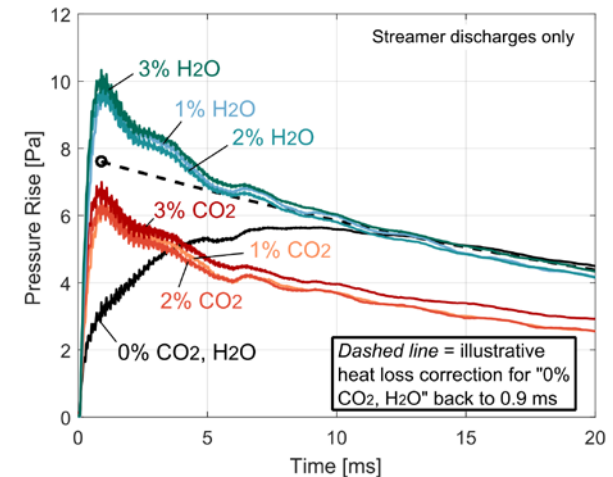
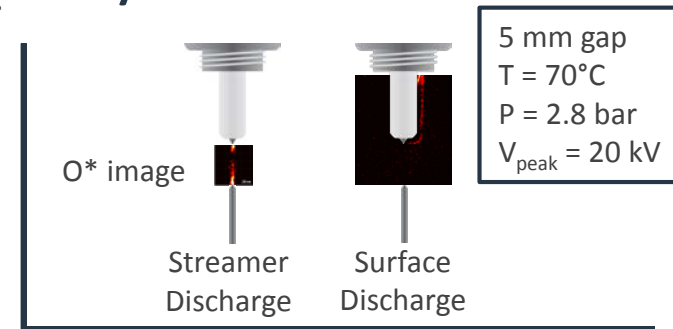
**Positive :** Sharper pressure-rise for streamer-only discharges indicates improved heating



**Negative :** Surface discharge probability increases with increased CO<sub>2</sub> or H<sub>2</sub>O content

- Surface discharge propensity is sensitive to insulator design

**Upshot:** Unknown chemical dynamics from CO<sub>2</sub> & H<sub>2</sub>O addition impact streamer behavior.



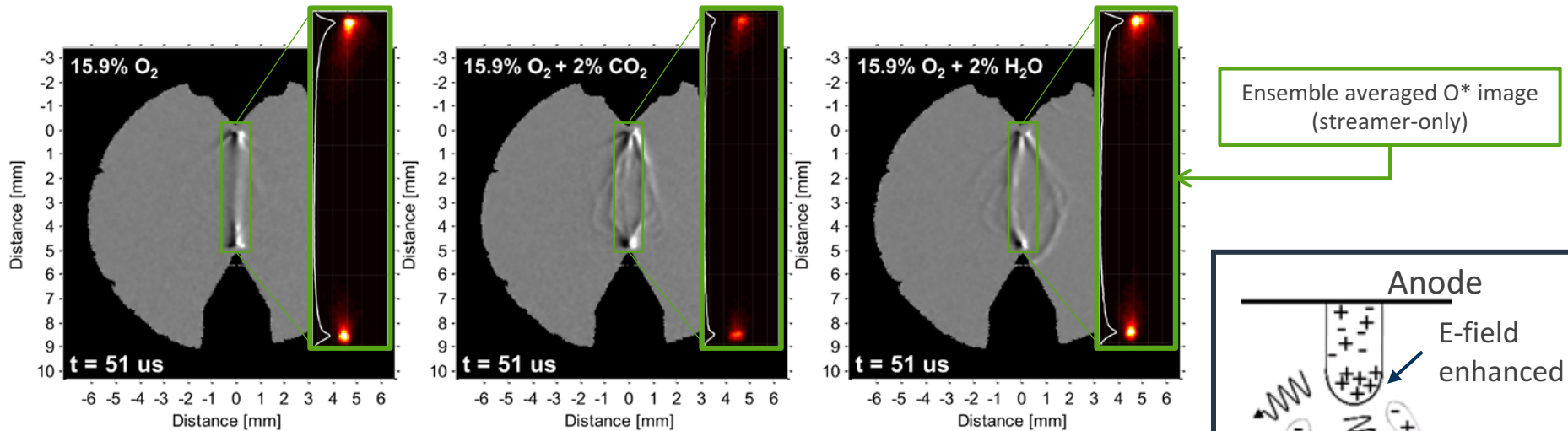
# Accomplishment: Unique dynamics with CO<sub>2</sub>/H<sub>2</sub>O explained

- CO<sub>2</sub> and H<sub>2</sub>O addition both lead to increased streamer branching

- Improved heating due to:

more branching → thin streamers → fast cooling → fast V-T relaxation

5 mm gap  
T = 70°C  
P = 2.8 bar  
V<sub>peak</sub> = 20 kV



- Decreased O\* formation with CO<sub>2</sub> addition
  - Not from changes in quenching, chemistry, or fluorescence trapping (see technical backup slides)
  - Likely from less E-field enhancement due to more efficient VUV CO<sub>2</sub> & H<sub>2</sub>O absorption relative to O<sub>2</sub>
  - **Not a feature of RF corona LTP due to the absence of VUV photons!**

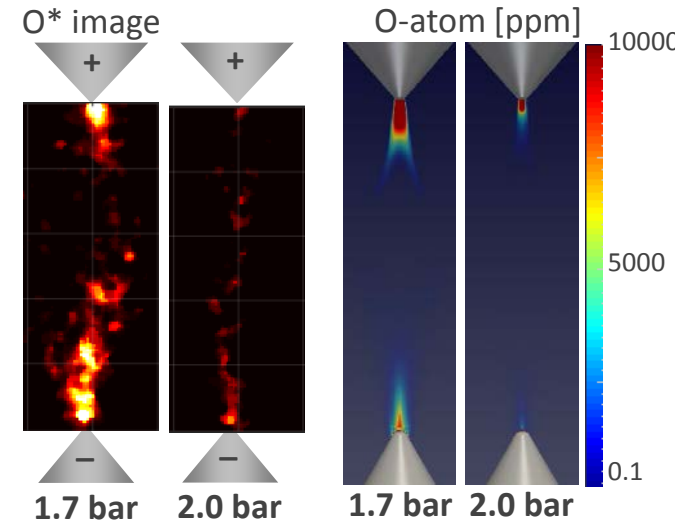
**Impact:** Unique nanosecond discharge streamer physics with CO<sub>2</sub> and H<sub>2</sub>O addition identified.



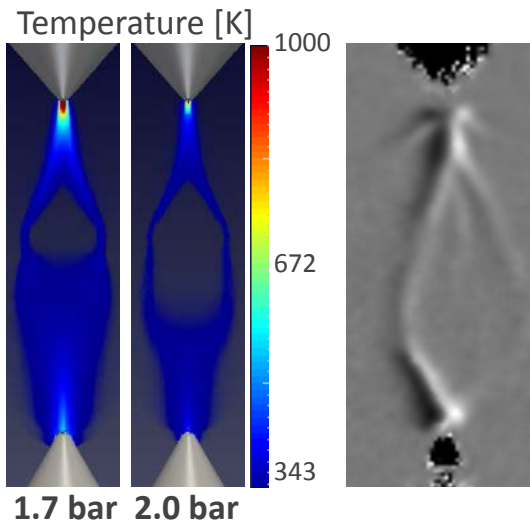
Basic Tests

# Accomplishment: LTP experiments & modeling comparison

- Substantial  $O^*$  observed for air nanosecond discharges  
 **$O(3p^3P \rightarrow 3s^3S)$  transition at 844.9 nm**
  - Due to high-energy electrons – not present w/ RF corona
  - Highest signal near electrodes where E-field is strongest
  - Rapid signal decrease w/ higher pressure due to lower E/N
- Argonne simulations show similar O-atom distributions
  - VizGlow: high-fidelity non-equilibrium plasma code that accounts for bulk-gas heating & photoionization effects



Simulation results courtesy of  
Riccardo Scarcelli  
Argonne National Laboratory



- Simulation temperature distributions also qualitatively agree with post-discharge schlieren images

**Impact: Complementary simulation & experiment capabilities enable systematic investigations into:**

- 1) the cause of surface discharges
- 2) best electrode configurations
- 3) optimal pulsing strategies

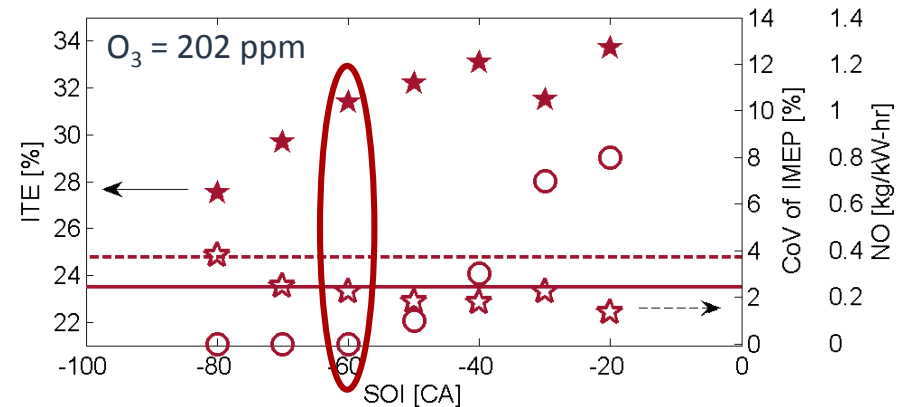
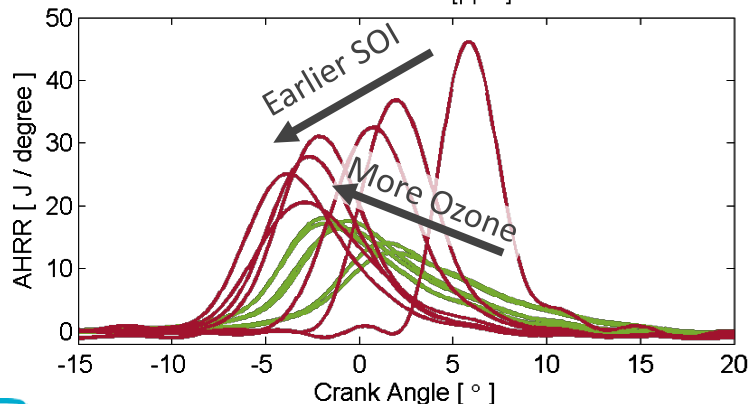
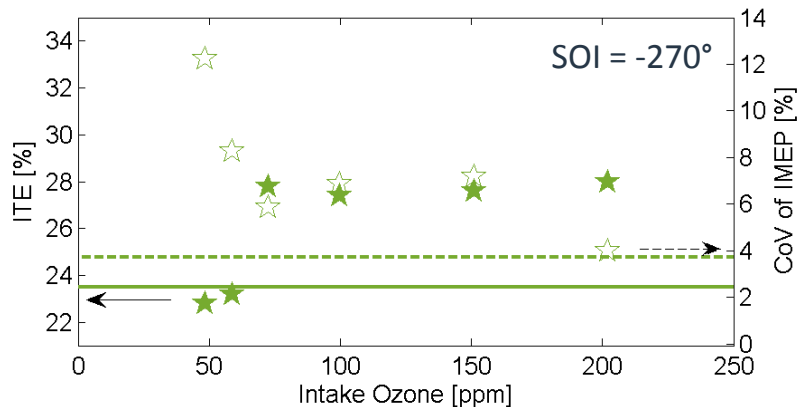


# Accomplishment: Characterization of $O_3$ on near-idle LTGC

## Controlled ozone concentrations seeded into the intake

- Goal: Benchmark engine performance with known quantities of  $O_3$ 
  - Will inform Q3 study where  $O_3$  is formed by the LTP discharge
- $\sim 80$  ppm  $O_3$  increases ITE  $\sim 5$  points relative to a similar NVO condition
  - Accelerated low-temperature chemistry advances combustion phasing

Speed: 1000 rpm  
Fuel: 6.2 mg/cycle  
(PRF 80)  
Load:  $\sim 1.5$  bar IMEP  
 $P_{\text{intake}}$ : 90 kPa  
 $T_{\text{intake}}$ : 155 K



- Further increase in ITE with DI retard
  - NO emissions rise for SOI retard beyond  $-50^\circ$  aTDC

**Impact:** Approx. 8 point ITE improvement relative to the best NVO operating point with virtually no NOx using ozone.



Engine Tests

# Reviewer Response

***Q1: Is the purpose of the ignition work to establish conditions for auto-ignition or initiate combustion.***

**Response:** We believe advanced ignition systems can switch between auto-ignition promotion for LTGC and flame propagation initiation for more conventional SI combustion on a cycle-resolved basis. Particular emphasis this year has been on nanosecond discharge LTP where non-thermal heating and radical production pathways can influence either mode of operation. Similar investigations for jet igniters are planned next year.

***Q2: Good explanation of observed effects of reformat addition, but progress continues to be slow.***

**Response:** A complete engine test-cell revamp along with the development of suitable optical diagnostics and complementary test vessels was required to properly address open questions about relevant advanced ignition systems. Now that these activities are mostly complete, research output related to advanced ignition systems has increased substantially.

***Q3: More OEM ignition system collaboration would help provide project guidance & industry feedback.***

**Response:** This past year we have reached out to various OEMs regarding collaborative ignition system testing and have also solicited project feedback. Most OEMs have provided guidance through intermittent video-conferences, phone calls, or informal conversations. We have a more active collaboration with GM R&D (that include shared hardware development) on turbulent jet ignition systems.

***Q5: Improved understanding of ignition systems and processes in gasoline engines is critical to improving engine efficiency.***

**Response:** We agree that new ignition systems enable more robust methods of operation that are not possible with more conventional ignition systems. The challenge continues to be devising high-value experiments that elucidate fundamental mechanisms so that these systems can be properly optimized.



# Collaborations

- National Lab
  - Argonne National Lab (Riccardo Scarcelli & James Sevik):
    - Shared validation data in support of advanced ignition modeling
  - Sandia FES (Ed Barnat & Matthew Hopkins):
    - Shared results and advice on LTP discharge modeling and experiments
- University
  - U. Orléans (Prof. Fabrice Foucher):
    - 3-month sabbatical by Prof. Fabrice Foucher to perform joint experiments into ozone formation by LTP discharges
  - Michigan State (Profs. Harold Schock & Elisa Toulson):
    - Joint jet ignition experiments with a common single-cylinder research head (w/ GM R&D)
  - U. Minnesota (Prof. William Northrop):
    - Assistance with in-cylinder reformat sampling
    - Reactor modeling of the reforming cycles
- Automotive OEM and Suppliers
  - GM R&D:
    - Regular technical interactions: 1) results exchange, 2) hardware support, & 3) feedback on research directions
    - Joint jet ignition experiments with a common single-cylinder research head (w/ Mich. State)
  - Ford, FCA, Cummings:
    - Intermittent technical discussion on LTP ignition: 1) results exchange & 2) feedback on research directions
  - Mahle GmbH:
    - Collaborative research on the mechanisms of ignition for jet ignition
    - Mahle to provide hardware loans as needed
- Small business
  - Transient Plasma Systems Inc.:
    - Data and hardware sharing
    - Electronics design and maintenance support for high-voltage nanosecond pulse generators
- DOE Working Group
  - Share research results and insights at the DOE's Advanced Engine Combustion working group meetings.

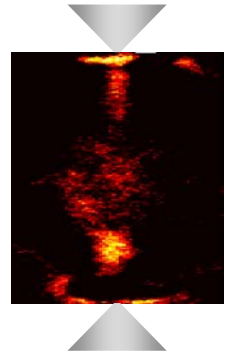




# Remaining Challenges and Barriers

- **LTP igniter design**: What are the optimal LTP igniter characteristics?
  - Is the cathode needed, or is an anode-only configuration sufficient?
  - Are higher voltages needed?
  - Can multi-pulse operation be used to increase heating while avoiding arc?
  - How can surface discharges be avoided? Insulator re-design?
- **In-cylinder ozone generation**: Can LTP generated  $O_3$  favorably influence LTGC auto-ignition?
  - Can  $O_3$  eliminate the need for intake pre-heating at very low loads?
  - What is the impact of added  $CO_2$ ? Does this reduce  $O_3$  formation rates?
  - Can multi-pulse be leveraged to increase radical yields?
- **Streamer initiated flame propagation**: Can nanosecond LTP non-thermal heating and radical production lead to extended dilution limits?
  - How do altered  $CO_2$  and  $H_2O$  streamer dynamics influence ignition? What about fuel?
  - Is there an in-cylinder density limitation?
- **Jet Ignition**: What are the mechanisms for ignition?
  - What is the interplay of flow (i.e., mixing) and chemistry on ignition?
  - How sensitive are ignition characteristics to what goes on in the pre-chamber?

Preliminary  $O_3$   
absorption image





# Future Work

Any proposed future work is subject to change based on funding levels

- **LTP igniter design:**

- Coat portions of electrode with high-dielectric strength epoxy to inhibit arc: **Q3FY17**
- Evaluate new TPS Inc. pulse generator capable of 50 kV<sub>peak</sub>: **Q4FY17**
- Identify supplier partners that can develop custom electrodes (i.e., insulators): **FY18**

- **In-cylinder ozone generation:**

- Measure LTP generated O<sub>3</sub> concentration in the calorimeter via laser absorption: **Q3FY17**
- Determine lowest intake temperature limit for stable low-load LTGC using O<sub>3</sub>: **Q3-Q4FY17**
- Explore impact of early-LTP on LTGC auto-ignition through O<sub>3</sub> formation: **Q3FY17-Q2FY18**

- **Streamer initiated flame propagation:**

- Perform additional LTP calorimetry and spectroscopic measurements with fuel, CO<sub>2</sub>, and H<sub>2</sub>O containing air mixtures: **Q3-Q4FY17 – Summer intern project**
- Explore impact of late-LTP on SI lean/dilute limits (w/ and w/o cathode): **Q3FY17-Q2FY18**
- With modelers, evaluate fast-gas heating & photoionization mechanisms: **Q3FY17-FY18**
- Find boosted SI operability limits with LTP: **Q4FY18**

- **Jet Ignition:**

- Assemble engine optimized for jet ignition: **Q3FY18**
- Visualize the chemical and mixing field at the jet head where ignition occurs: **FY18**



# Summary

## Relevance

- Explore how advanced ignition systems can facilitate efficient, mixed-mode combustion across the load/speed map: i.e., low-load LTGC, moderate-load dilute SI, and high-load boosted SI.

## Approach

- Remove new igniter commercialization barriers through targeted engine and optical calorimetry experiments, with complementary modeling performed by national lab partners

## Technical Accomplishments

- In-cylinder generated reformat can optimally phase LTGC auto-ignition through altered fuel reactivity characteristics – Parasitic heat loss penalty (4 – 6% of the fuel energy) makes this strategy prohibitive
- Arc transition probability mapped for nanosecond discharges at engine relevant densities for mixtures of air, CO<sub>2</sub>, and H<sub>2</sub>O using canonical pin-to-pin electrodes

- CO<sub>2</sub> and H<sub>2</sub>O found accelerate bulk-gas heating due to thinner streamers, but increased the propensity for surface discharges due to interrupted photoionization processes
- Argonne simulations (VizGlow) found to qualitatively agree with discharge imaging
- Thermal arc transition mechanism for multi-pulse nanosecond discharge operation identified
- ~80 ppm of O<sub>3</sub> addition found to effectively phase LTGC auto-ignition and led to an ~8 point improvement in ITE relative to NVO operation due to a reduction in heat losses

## Proposed Future Research

- Optimize LTP discharge igniter geometry
- Experimentally explore in-cylinder O<sub>3</sub> production via LTP on LTGC
- Measure streamer dynamics in the optical spark calorimeter and evaluate LTP on lean/dilute SI
- Build and test engine outfitted with a jet igniter

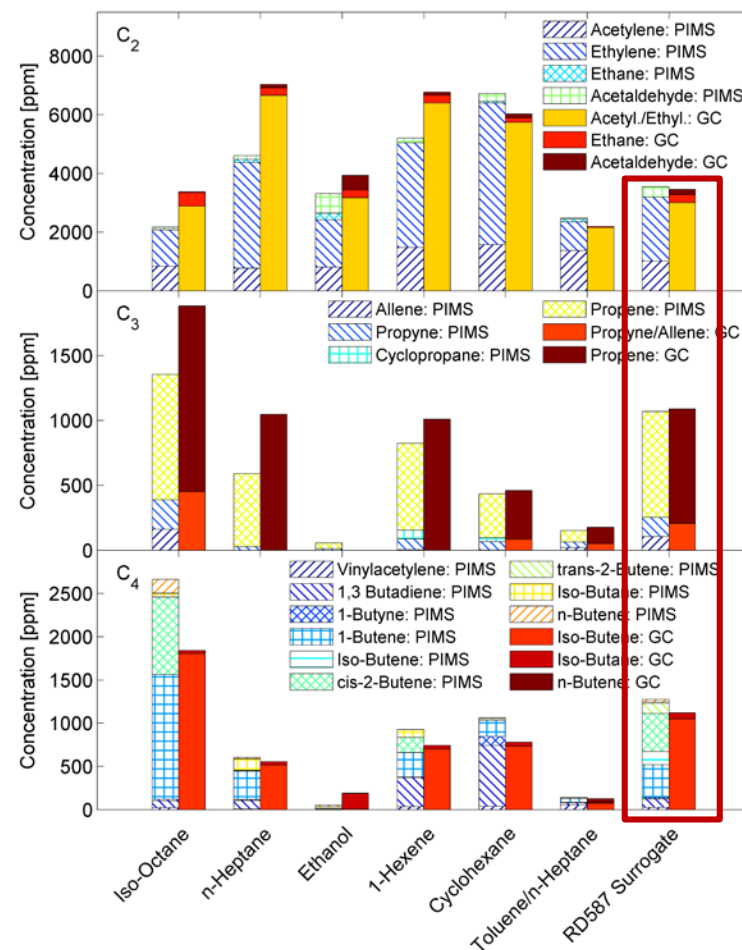
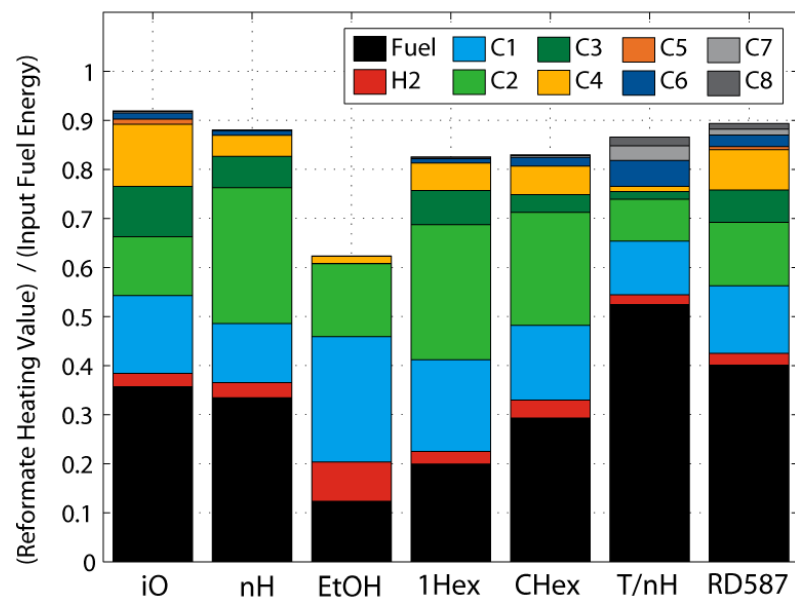


Any proposed future work is subject to change based on funding levels

# Technical Backup Slides

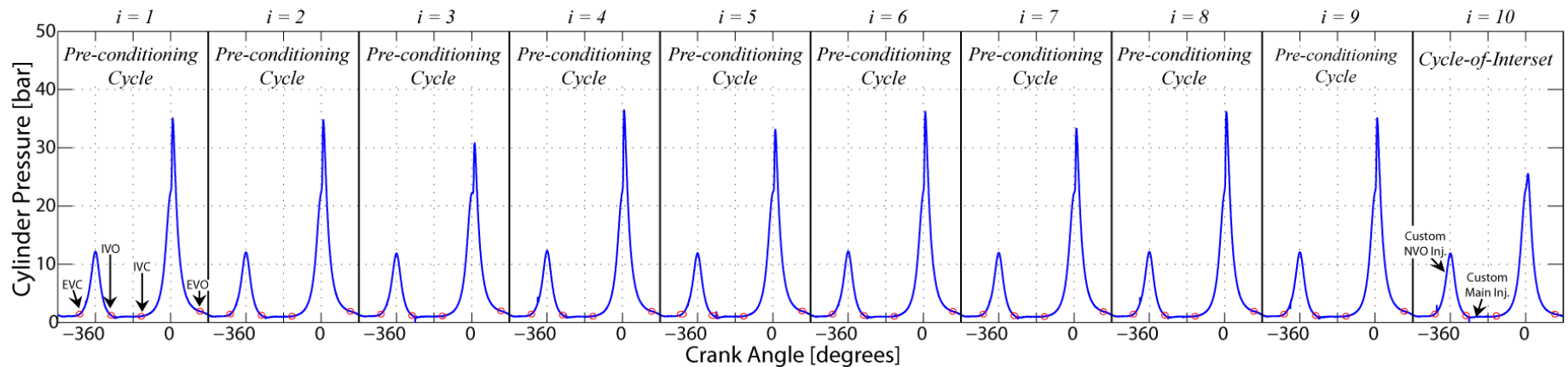
# Technical Backup Slide: Reformate Constituents

- **GC:** characterize fuel energy breakdown
  - ~90% fuel energy recovery (~60% for ethanol)
  - most energy from parent fuel, CO, H<sub>2</sub>, & small HC
- **PIMS:** find species that influence auto-ignition
  - higher fidelity speciation relative to GC results



**Impact:** Results enable a systematic evaluation into the importance of each constituent on auto-ignition chemistry via kinetic modeling.

# Technical Backup Slide: Alternate-fire cycle energy model



Includes retained exhaust enthalpy & fuel

Woschni correlation

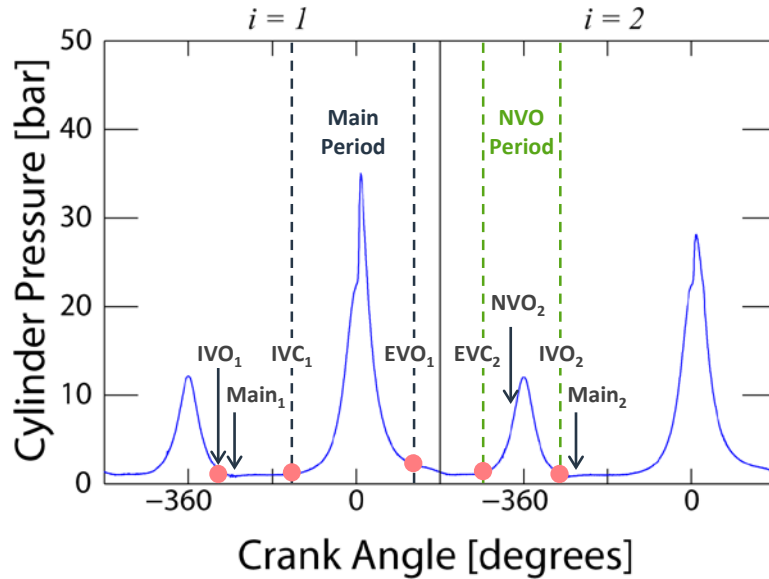
$$U_{input_i} = W_i + Q_{HT_i} + H_{EVO_i} + U_{fuel,EVO_i}$$

Unsteady exhaust composition limits direct measurement

$\int PdV$   $f(m_{EVO}, T_{EVO}, \chi_{EVO})$

Solving each term requires estimates of the: (1) residual gas fraction, (2) composition at each valve event & (3) bulk-gas temperature

# Technical Backup Slide: Alternate-fire cycle energy model



$$1. \quad RGF_i \equiv \frac{\sum_j m_{NVO,out,i,j}}{\sum_j m_{main,out,i-1,j}}$$

$$2. \quad \sum_j m_{main,in,i-1,j} = \sum_j m_{int,j} + \sum_j m_{NVO,out,i-1,j}$$

$$3. \quad \sum_j m_{main,out,i-1,j} = \sum_j m_{main,in,i-1,j} + m_{main,i-1,fuel}$$

$$4. \quad \sum_j m_{exh,i-1,j} = \sum_j m_{int,j} + m_{main,i-1,fuel} + m_{NVO,i-1,fuel}$$

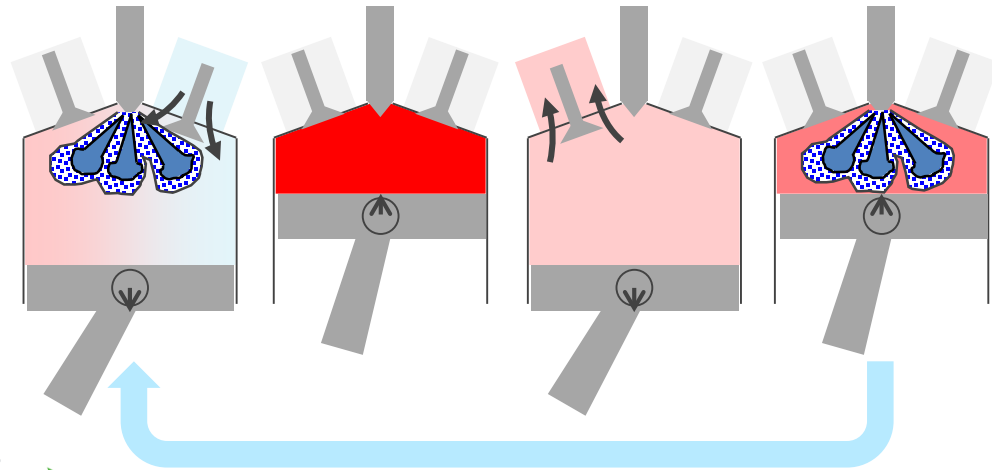
$$5. \quad \sum_j m_{NVO,in,i,j} = \sum_j m_{main,out,i-1,j} - \sum_j m_{exh,i-1,j}$$

$$6. \quad \sum_j m_{NVO,out,i,j} = \sum_j m_{NVO,in,i,j} + m_{NVO,i,fuel}$$

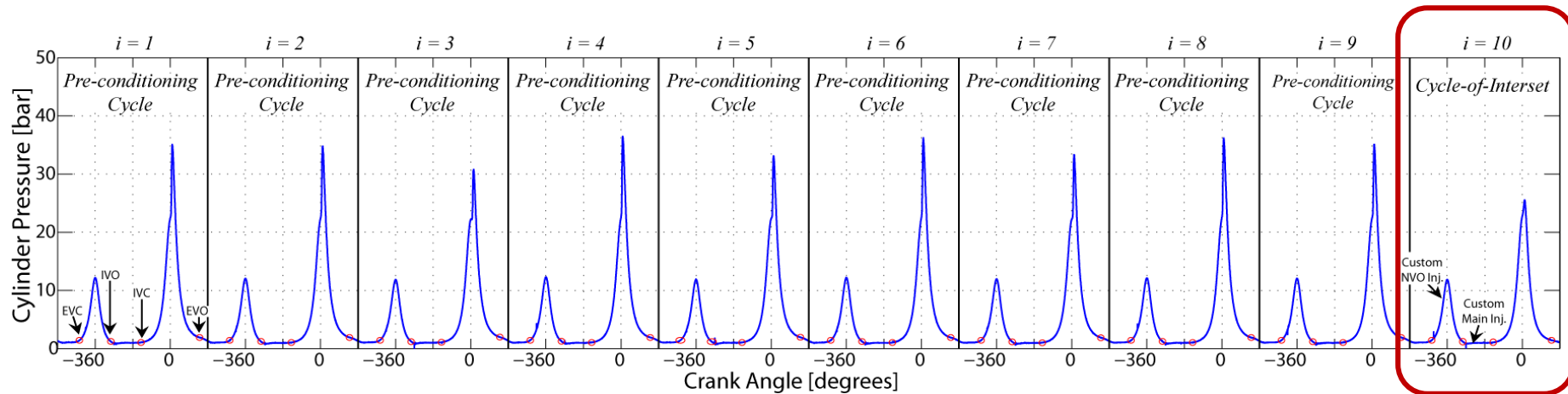
## Composition out of Main and NVO-periods

- 6 species considered:  $j = N_2, O_2, CO_2, H_2O, CO, fuel$ 
  - 4 atom balance eqns. for each NVO & main period
- Closed Main period** assumptions:
  - All fuel consumed (globally lean)
  - 95% of fuel carbon to  $CO_2$ ; 5% to CO
- Closed NVO period** assumptions:
  - All  $O_2$  consumed (globally rich)
  - 90% of fuel carbon converted to CO; 10% stays as fuel

Bulk-temp. solved using trapped mass & cyl. press.

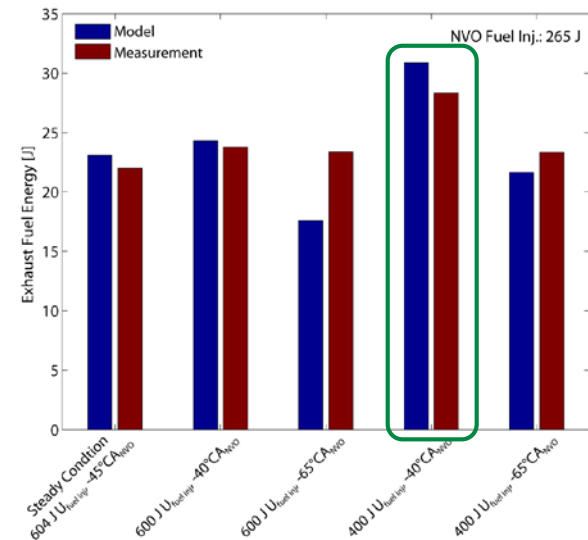


# Technical Backup Slide: Alternate-fire cycle energy model

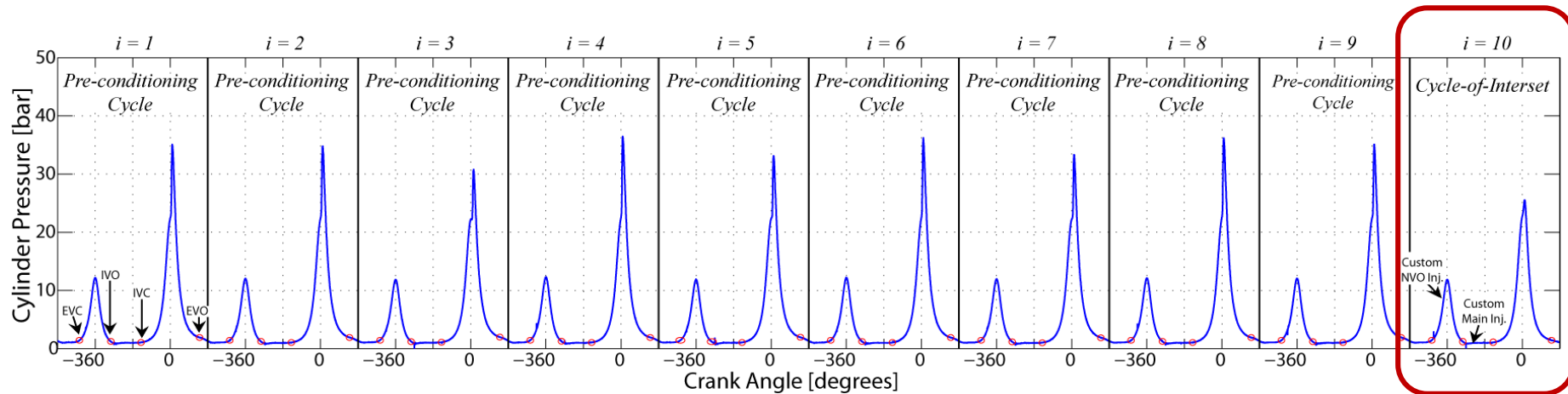


$$U_{input_i} \equiv U_{fuel\ inj_i} + (H + U_{fuel})_{EVC_i} - (H + U_{fuel})_{EVC_{i+1}} = W_i + Q_{HT_i} + H_{exh_i} + U_{fuel,exh_i}$$

- Model exhaust fuel energy values compare favorably to dump-sample measurements

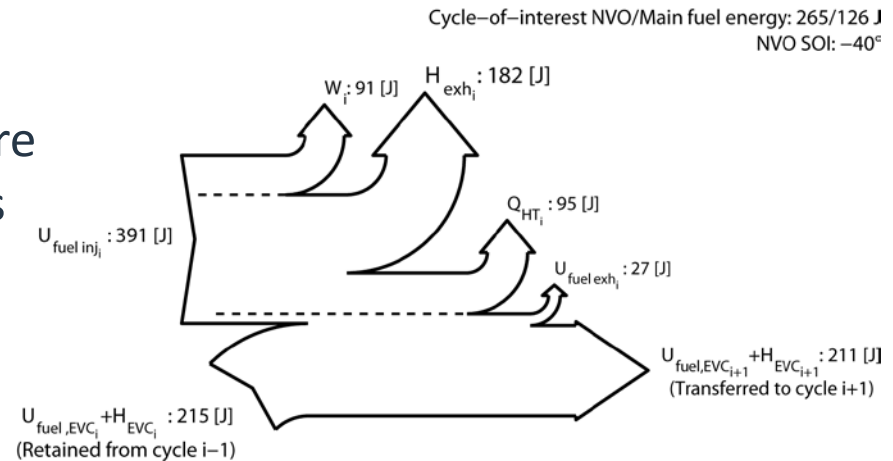


# Technical Backup Slide: Alternate-fire cycle energy model



$$U_{input_i} \equiv U_{fuel\ inj_i} + (H + U_{fuel})_{EVC_i} - (H + U_{fuel})_{EVC_{i+1}} = W_i + Q_{HT_i} + H_{exh_i} + U_{fuel,exh_i}$$

- Model exhaust fuel energy values compare favorably to dump-sample measurements
- Similar input and output energy flows





# Technical Backup Slide: Argonne engine experiments

NGK  
Conventional Spark



## Current Focus

TPS Inc.  
Close-Coupled PND

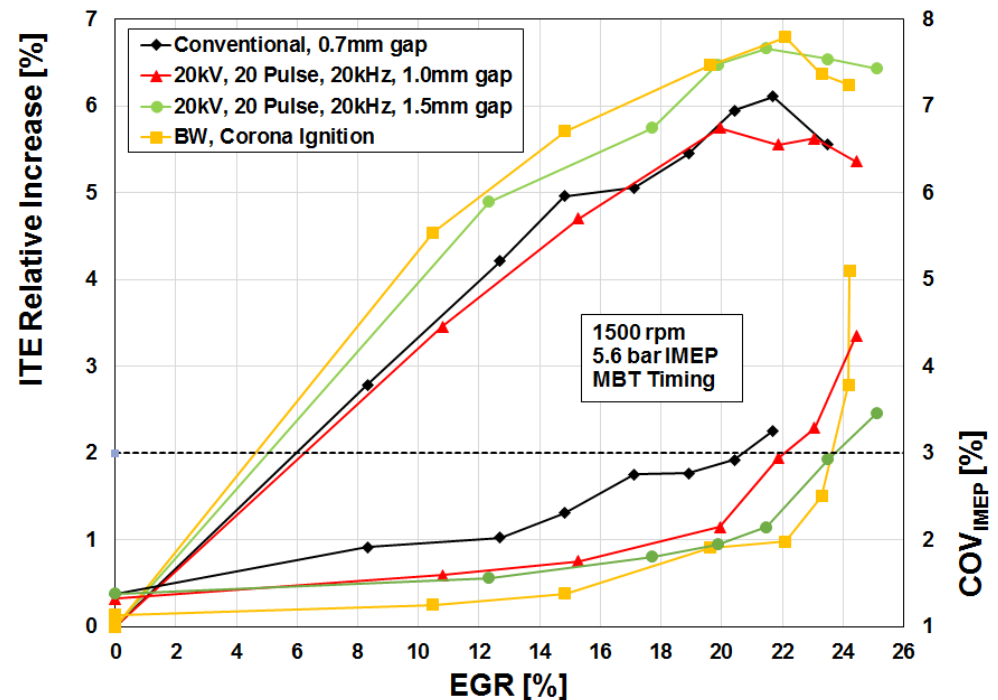


BorgWarner  
EcoFlash RF Corona



Displacement	0.6 L
Bore x Stroke [mm]	89.04 x 100.6
Compression Ratio	12.1:1

Similar results found  
for lean operation



- What is the ignition mechanism?
- How does EGR influence discharge phenomena?
- What prevents further dilution limit extension?

# Technical Backup Slide: LTP discharge phases

## 1. Primary streamer phase

+ 10's of kV



**Ionization by primary streamer head.**  
Electrons move towards anode leaving positive space charge in streamer path.



$\Delta t \sim \mathcal{O}(1 \text{ ns})$

- GND

## 2. Compensation phase

+



**Primary streamer connects to cathode.**  
Negative charge flows from cathode to compensate positive space charge.  
E-field increases near anode.

-

## 3. Secondary streamer phase

**LTP**

+



**Secondary streamer advances.**  
Strong E-field near anode leads to rapid advance.



$\Delta t \sim \mathcal{O}(10 \text{ ns})$

-

**SSB**

## 4. Transient arc phase

+



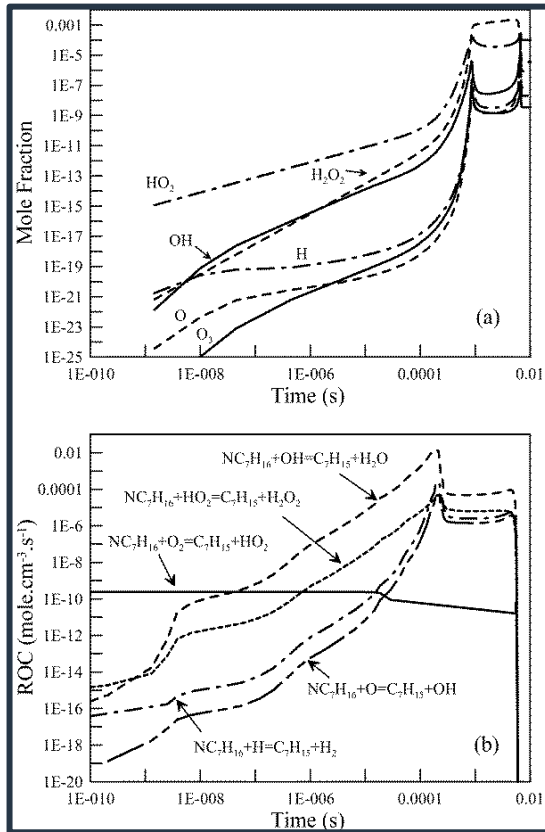
**Arc occurs if secondary streamer reaches cathode ( $E/N$  high along the entire discharge filament).**  
Secondary streamer propagation promoted by local heating from V-T relaxation (reduction in  $N$ ).

-

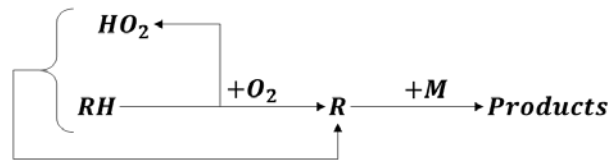
Marode, J. Appl. Phys., 1974;46(5).  
Bastien & Marode, J. Phys. D: Appl. Phys., 1985; 18(377).

Close-coupled PND (100  $\mu\text{s}$  dwell) aim to increase **radical formation** while ideally **avoiding secondary streamer breakdown (SSB)**

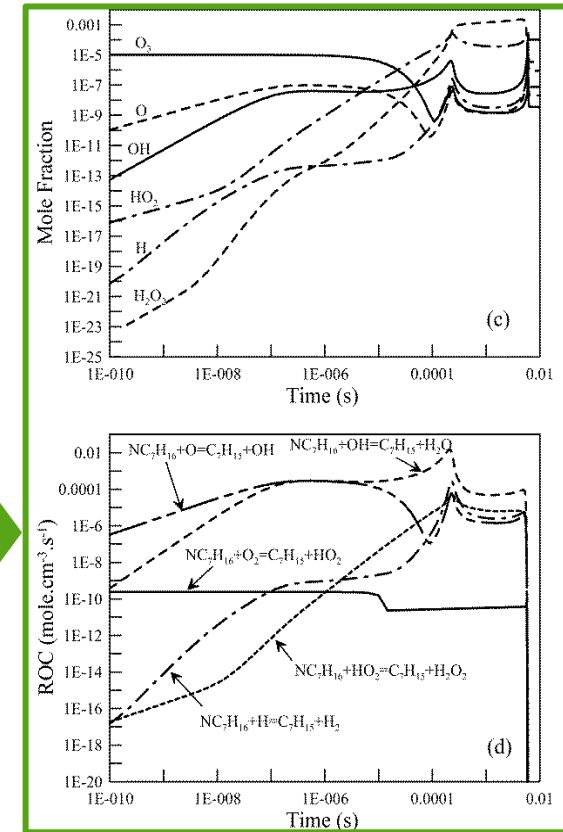
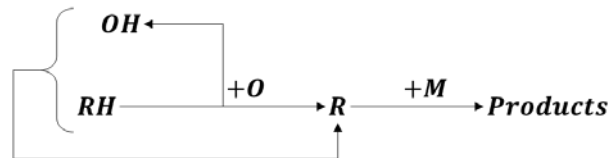
# Technical Backup Slide: Impact of O-atom on LTHR



Without ozone

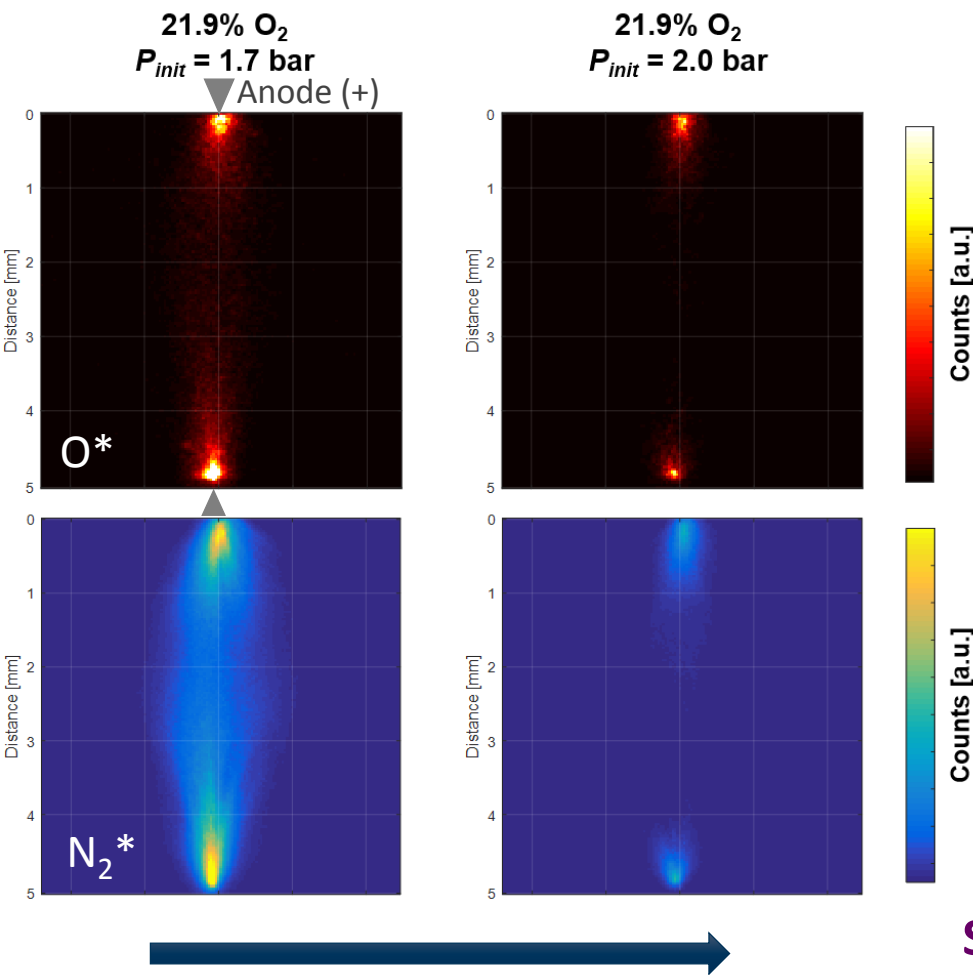


With ozone



Uncertain kinetic modeling at engine relevant conditions

# Technical Backup Slide: Influence of pressure on emission



## O\*: O(3p<sup>3</sup>P → 3s<sup>3</sup>S) at 844.9 nm

- Image intensity changed -61% for  $\uparrow P_{init}$ 
  - Estimated change in fluorescence quantum yield (FQY) = -15%

## N<sub>2</sub>\*: N<sub>2</sub>(C<sup>3</sup>Π<sub>u</sub> → B<sup>3</sup>Π<sub>g</sub>) at 337.1 nm

- Image intensity changed -75% for  $\uparrow P_{init}$ 
  - Est. change in FQY = -15%

Suggests other factor important, e.g. E/N

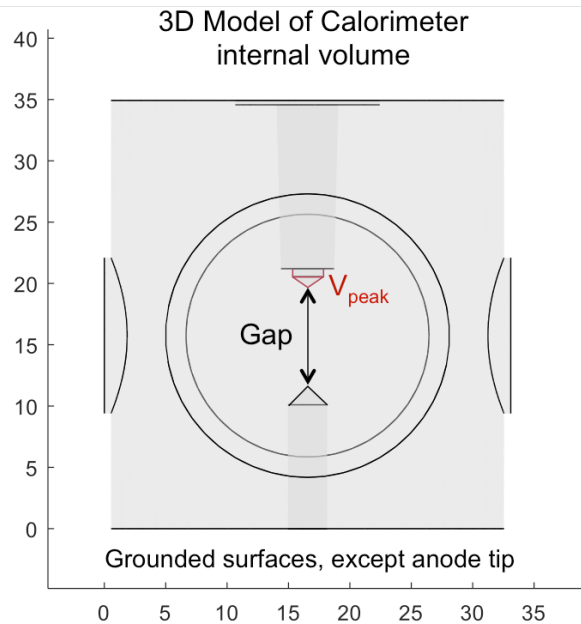


Single pulse  
Top = O\*: 500 ns gate  
Bottom = N<sub>2</sub>\*: 500 ns gate



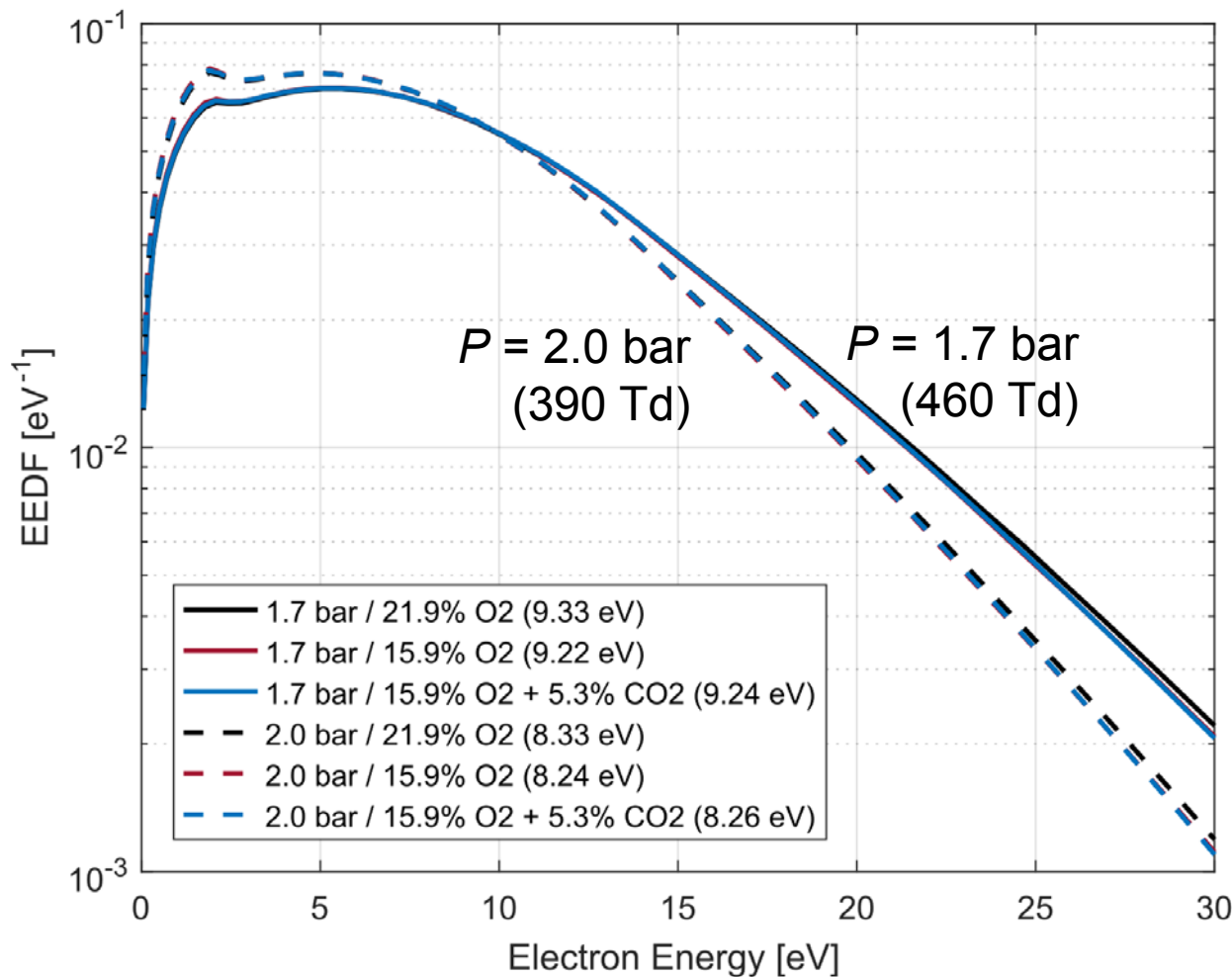
# Technical Backup Slide: Estimated LTP EEDF

## MATLAB model to estimate E/N



## BOLSIG+ to estimate EEDF

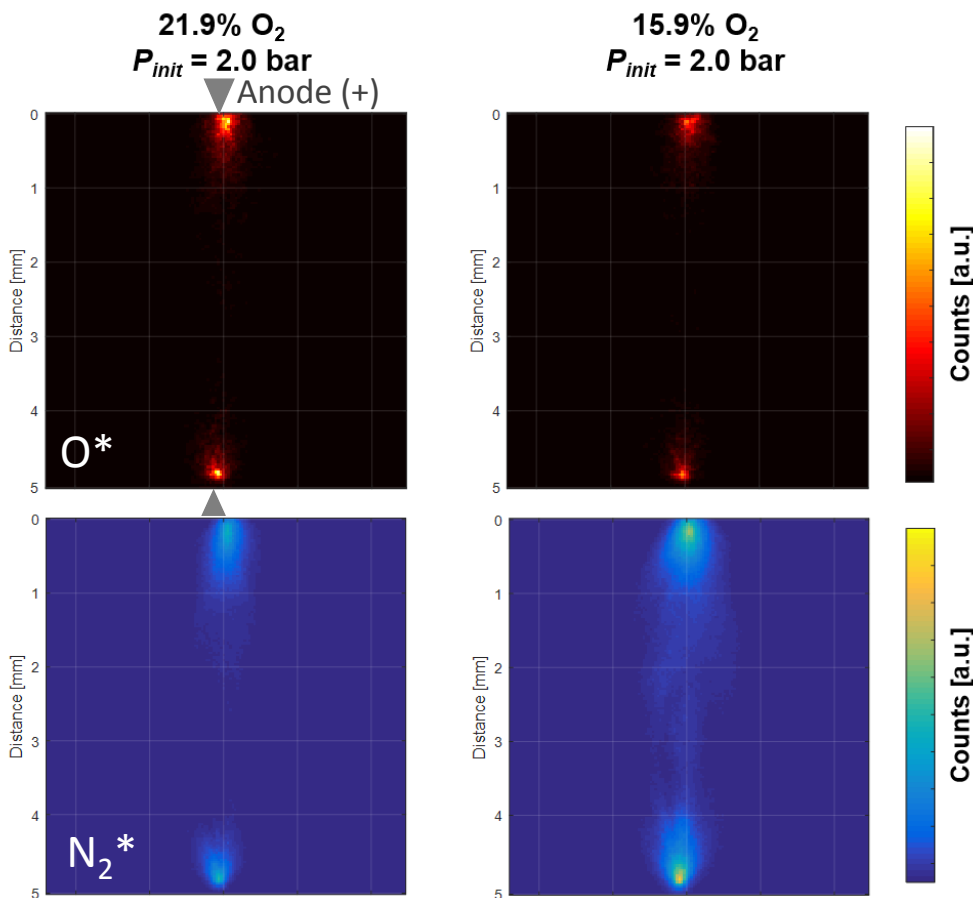
E/N, composition, temperature, and collision cross-sections of  $O_2$ ,  $N_2$ ,  $CO_2$  (attachment, elastic, rot./vib. excitation, ionization)



Impact of increased pressure may be explained by EEDF

Note: impact of pressure > impact of gas composition

# Technical Backup Slide: Influence of O<sub>2</sub> on emission



## O\*: O(3p<sup>3</sup>P → 3s<sup>3</sup>S) at 844.9 nm

- Image intensity changed **-27%** for ↓X<sub>O<sub>2</sub></sub>
  - Estimated change in FQY = +4%
  - Change in X<sub>O<sub>2</sub></sub> = -28%
  - Total est. change = **-24%**, agrees well

## N<sub>2</sub>\*: N<sub>2</sub>(C<sup>3</sup>Π<sub>u</sub> → B<sup>3</sup>Π<sub>g</sub>) at 337.1 nm

- Image intensity changed **+85%** for ↓X<sub>O<sub>2</sub></sub>
  - Estimated change in FQY = +30%
  - Change in X<sub>N<sub>2</sub></sub> = +8%
  - Total est. change = **+38%**, right trend
  - Note: single transition not isolated

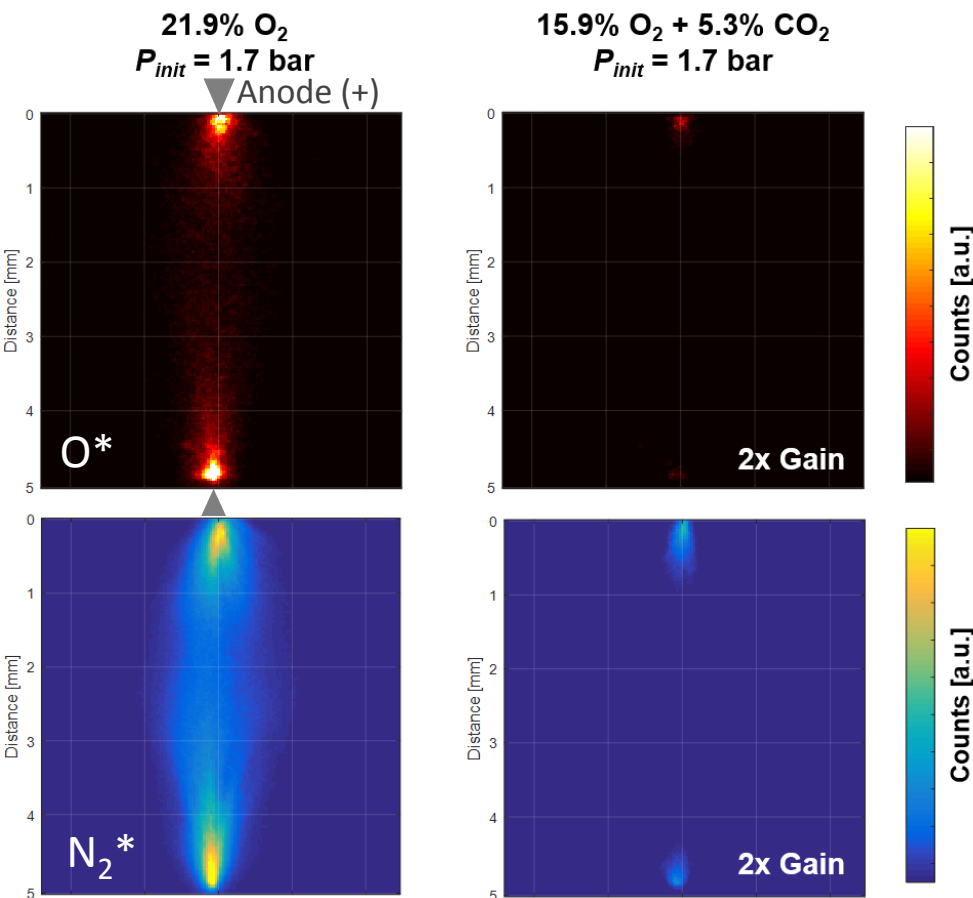
Decreasing X<sub>O<sub>2</sub></sub> at constant pressure



Single pulse  
Top = O\*: 500 ns gate  
Bottom = N<sub>2</sub>\*: 500 ns gate



# Technical Backup Slide: Influence of CO<sub>2</sub> on emission



## O\*: O(3p<sup>3</sup>P → 3s<sup>3</sup>S) at 844.9 nm

- Image intensity changed **-92%** for  $\uparrow X_{CO_2}$  &  $\downarrow X_{O_2}$ 
  - Estimated change in FQY = +3%
  - Change in O<sub>2</sub> conc. = -28%
  - Total est. change = **-25%**, does not agree

## N<sub>2</sub>\*: N<sub>2</sub>(C<sup>3</sup>Π<sub>u</sub> → B<sup>3</sup>Π<sub>g</sub>) at 337.1 nm

- Image intensity changed **-91%** for  $\downarrow P_{init}$ 
  - Estimated change in FQY = -4%
  - No change in N<sub>2</sub> conc.
  - Total est. change = **-4%**, does not agree
  - Note: single transition not isolated

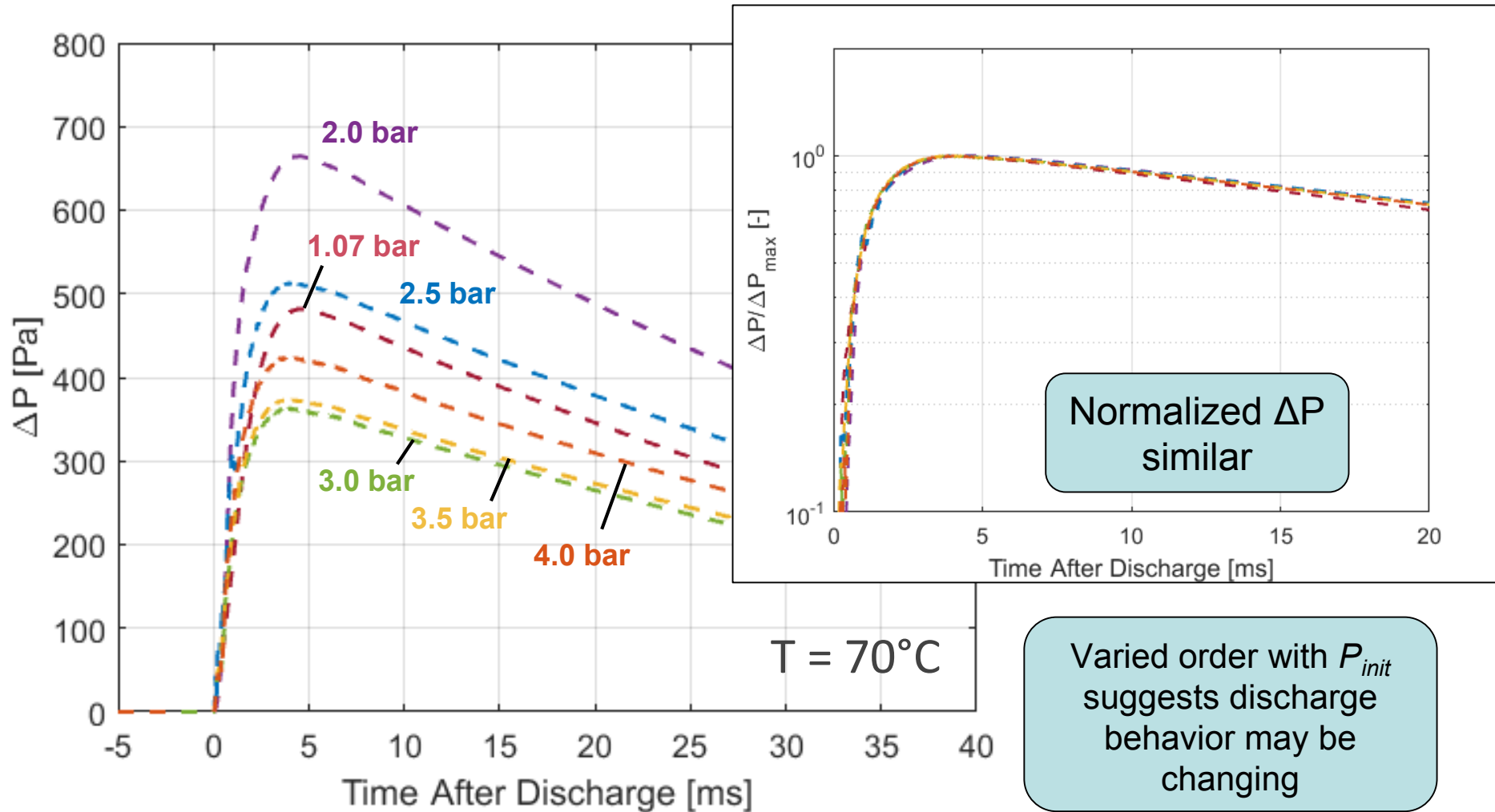
Increasing  $X_{CO_2}$  at constant pressure



Single pulse  
Top = O\*: 500 ns gate  
Bottom = N<sub>2</sub>\*: 500 ns gate

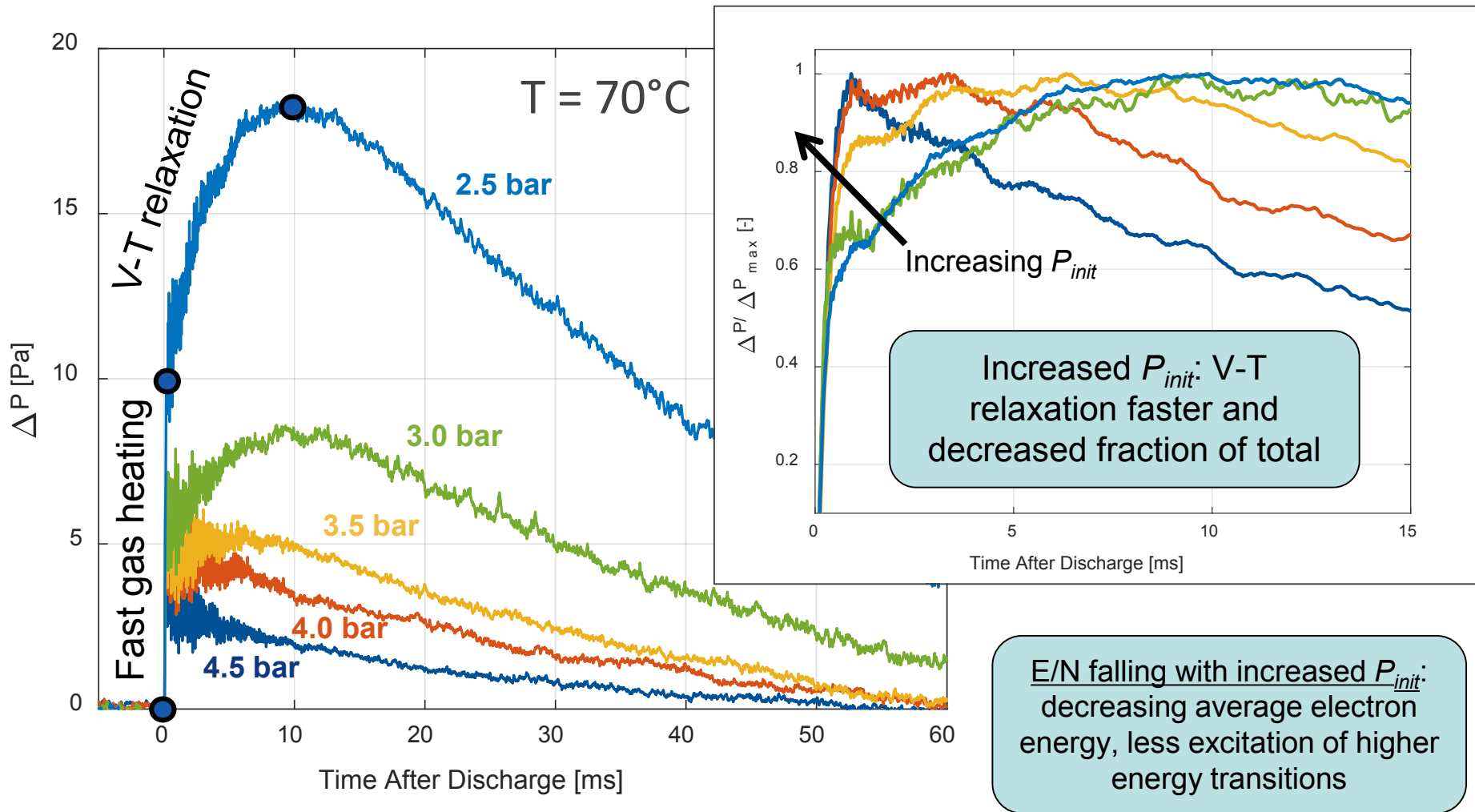
- Impact of CO<sub>2</sub> not explained by EEDF, quenching (or fluorescence trapping)
- Kinetics? ANL modeling effort.

# Technical Backup Slide: Pressure calorimeter – arc

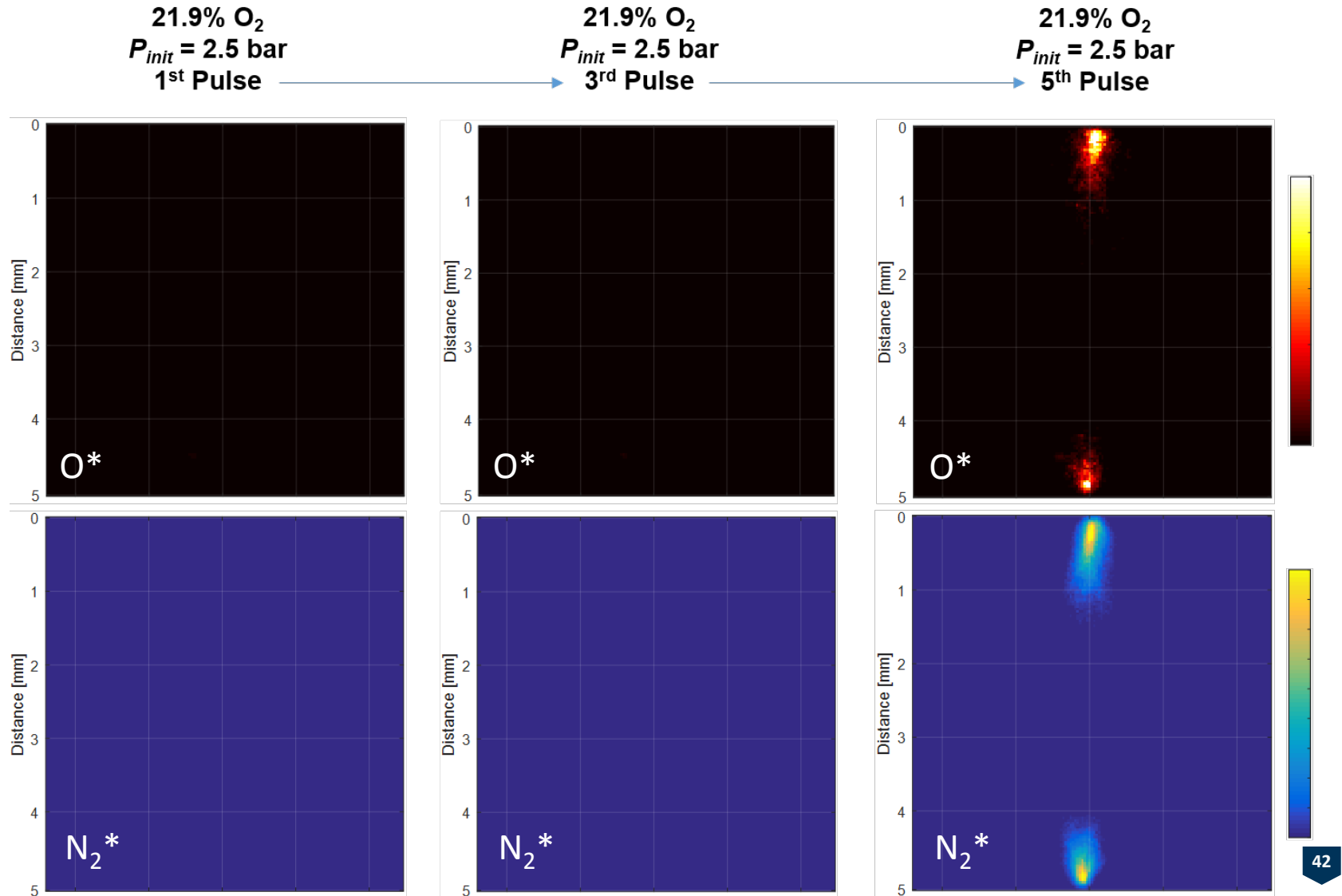




# Technical Backup Slide: Pressure calorimeter – LTP

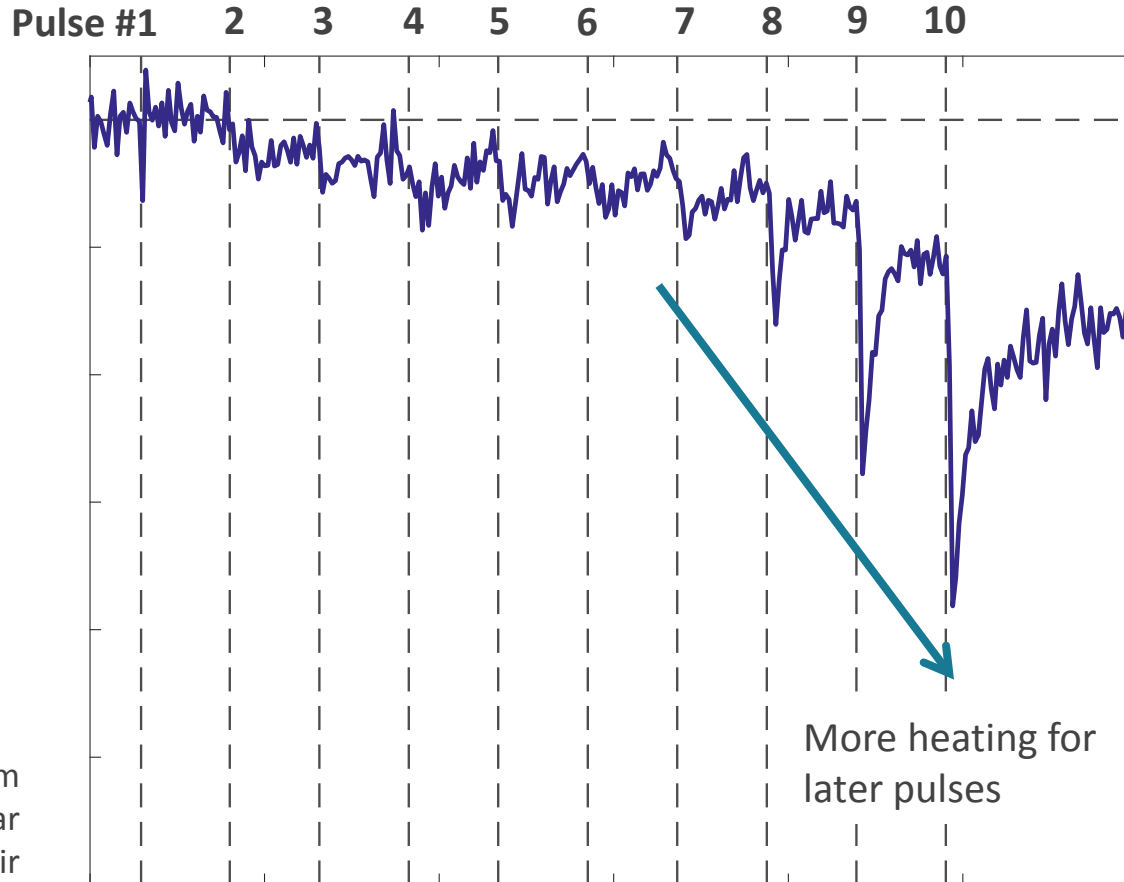


## Technical Backup Slide: Emission with multi-pulse



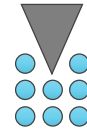
# Technical Backup Slide: Argonne APS x-ray radiography

Conditionally-averaged on LTP-only discharges  
(42.5% of total runs)

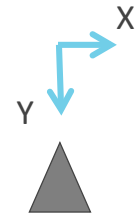


Gap = 3 mm  
 $P = 4.34$  bar  
Ultra air

Anode (+)



8 probe points x  
120 runs/point  
 $\Delta y = 100 \mu\text{m}$   
 $\Delta x = 75 \mu\text{m}$

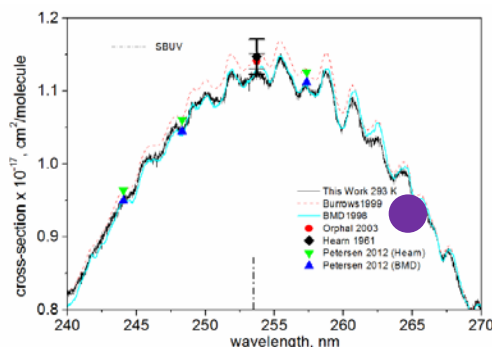
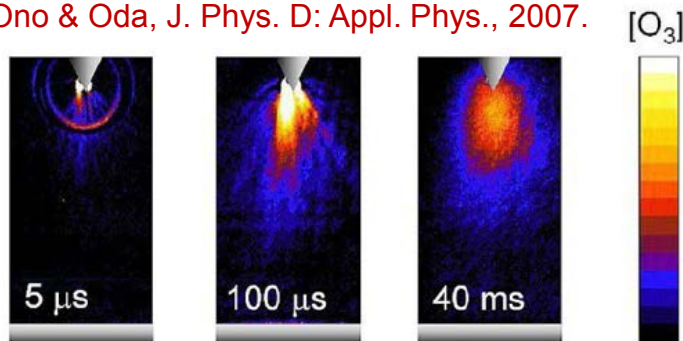


Cathode (GND)

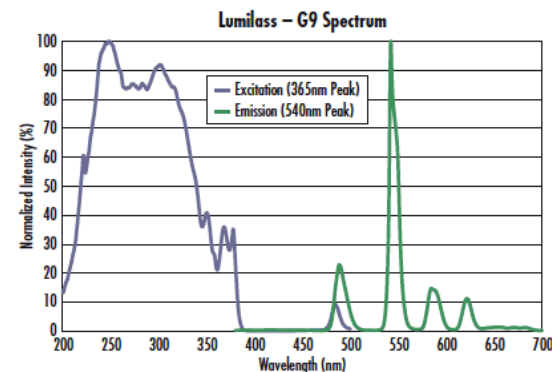
Measurements by:  
A. Kastengren  
D. Duke  
K. Matusik

# Technical Backup Slide: Ozone laser absorption

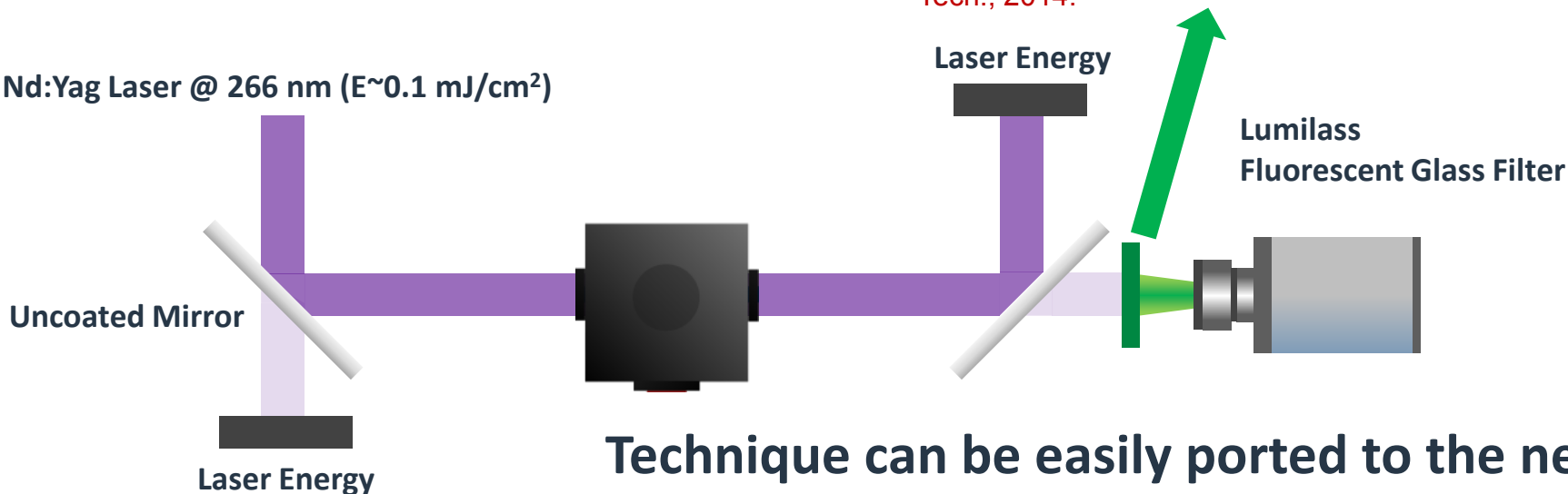
Ono & Oda, J. Phys. D: Appl. Phys., 2007.



Gorshlev et al., Atmos. Meas. Tech., 2014.



Nd:Yag Laser @ 266 nm ( $E \sim 0.1$  mJ/cm<sup>2</sup>)



Technique can be easily ported to the new optically-accessible gasoline research engine